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CRS4

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**On the representation of incompressible  
Newtonian free-surface CFD flows**

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## Abstract

This paper presents an attempt to develop a comprehensive representation of two components incompressible Newtonian flows. The primary target is to have insight on how to improve the CFD simulations of free-surface flows so as to deal with very high density ratios. First, the Navier-Stokes equations of a fluid with two immiscible components is derived from the single component equations. In this case, the surface tension does not come from the equations and must be added externally. Second we shortly review the Cahn-Hilliard and Allen-Cahn equations describing a phase separation process, and the phenomenological relation with surface-tension phenomena.

Third, we build phase momentum equations which are consistent with the classical Navier-Stokes equations, but this time for miscible fluids. The concept of energy conservation applied separately to the phases is systematically used to build the phase momentum forces, with a particular regard to the surface tension. Fourth, by use of a dynamical equilibrium assumption and a specific splitting of the energies and their derived force, we retrieve the basic properties of the phase transport equations. The method is extended to the surface tension and to the baro-diffusion. The relation between the phase forces and diffusion fluxes is clarified. Finally, a complete and consistent set of equations is provided and discussed.

## Contents

<b>1</b>	<b>Introduction</b>	<b>3</b>
<b>2</b>	<b>System of equations for two immiscible fluids</b>	<b>5</b>
<b>3</b>	<b>On surface tension and immiscibility</b>	<b>11</b>
3.1	Cahn-Hilliard equation . . . . .	11
3.2	Allen-Cahn equation . . . . .	12
3.3	Representation of the surface tension . . . . .	13
3.4	Derivation of the surface tension from energy consideration . .	14
<b>4</b>	<b>System of equations for two miscible fluids</b>	<b>16</b>
4.1	Momentum equation . . . . .	17
4.2	Inter-phase momentum transfer . . . . .	21
4.3	Volume fraction equation . . . . .	22
<b>5</b>	<b>Energy consideration</b>	<b>23</b>
5.1	Derivation of standard diffusion from energy consideration . . .	24
5.2	Gravitational potential . . . . .	25
5.3	Pressure shift . . . . .	26

<b>6</b>	<b>Dynamic equilibrium assumption</b>	<b>28</b>
6.1	Extension to other internal phenomena . . . . .	30
6.2	Extension of the derivation of the surface tension from energy consideration . . . . .	32
6.3	Extension of the notion of surface density . . . . .	36
6.4	Relation between potentials . . . . .	38
6.5	Relation with the Cahn-Hilliard equation . . . . .	39
<b>7</b>	<b>Consequences for the numerical treatment of surface tension</b>	<b>40</b>
<b>8</b>	<b>Final system of equation</b>	<b>43</b>
<b>9</b>	<b>Discussion</b>	<b>44</b>
<b>10</b>	<b>Formula</b>	<b>46</b>
<b>11</b>	<b>Acknowledgments</b>	<b>47</b>

# 1 Introduction

This work has been performed in the framework of the European Union THINS <sup>1</sup> project. We report hereafter the first paragraph of the project description.

“For the long-term development of nuclear power, innovative nuclear systems such as Gen-IV reactors and transmutation systems need to be developed for meeting future energy challenges. Thermal-hydraulics is recognized as a key scientific subject in the development of innovative reactor systems. This project is devoted to important cross-cutting thermal-hydraulic issues encountered in various innovative nuclear systems, such as advanced reactor core thermal-hydraulics, single phase mixed convection and turbulence, specific multiphase flow, and code coupling and qualification.”

Our part in the project deals with free-surface flows CFD simulations with commercial software, here Starccm+ from CD-Adapco. With this software, it is now possible to perform meaningful simulations in the VOF formulation. It is in continuous improvement so it is useful to follow the progress and have a clear idea of the possible applications. There are however some fundamental limitations that we would like to eliminate, at least try to.

In effect, playing with the software, it turns out that it is almost impossible (at least for the author) to stabilize a CFD simulation of a two-phase flow with a ratio of density decisively larger than the usual water-air density ratio at 1 Bar. We need however to deal with heavy liquid metal flows in contact with gas at atmospheric, or even much lower, pressure. Another encountered defect is that when a free-surface is subject to the combined effect of shear and oscillation, then it begins to non-physically diffuse. This effect has been encountered while trying to simulate a tentative design of a windowless target for MYRRHA<sup>2</sup>. In this design, a liquid Lead-Bismuth Eutectic LBE presents a free-surface towards an upper almost vacuum. It is therefore completely non-physical to interpret phase mixing in this context as bubble inclusions. The issue was readily solved by adding a surface sink of the light phase at the interface. The almost vacuum was simulated as an incompressible fluid with density about 10, to comply with the density ratio constraint. While the windowless MYRRHA target option has been discarded, we still have to model LBE flows, however, in contact with a cover gas at ambient pressure. In effect, LBE serves as primary coolant of MYRRHA. The density ratio then becomes an issue because in the future we would like to be able to

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<sup>1</sup>Thermal-hydraulics of Innovative Nuclear Systems, Funded under 7th FWP, project ref. 249337

<sup>2</sup>[www.iaea.org/inisnkm/nkm/ws/d2/r1655.html](http://www.iaea.org/inisnkm/nkm/ws/d2/r1655.html)

understand the combined dynamic of the LBE/cover gas flow, comprehensive of possible pollutants diffusion. A correct description of the gas will become more critical and so will be the density ratio issue. To be able to follow the diffusion of pollutants across the free-surface, we also definitively need to have a sharpening algorithm which is fully conservative. In this context, we also observed that where the free-surface is stagnant (heavy liquid side) then a relatively large parasite un-physical flow fields develops at the light phase side, and this independently of any applied surface tension.

The idea behind this work is that the density ratio issue, the parasite flow and the surface smearing are different aspects of the same problem. It is very common, to explain free-surface smearing, to invoke errors from the discretisation, from the convection or the temporal numerical schemes. The result is that the surface smearing is contrasted with numerical schemes adaptation. Our feeling is that the core of the problems may also lie inside the set of solved equations. We therefore want to derive a set of equations whose numerical resolution should naturally give a sharp interface when it is due. For this, we must understand more deeply how the Navier-Stokes equations are derived and why gases mix but liquids often do not. This work is rather theoretical in nature and is propaedeutic to a future numerical implementation.

The paper is organized as follows. We derive the most rigorously as we can the unclosed equations of a flow composed of two immiscible fluids. This derivation in some sense generalizes and simplifies the first part of the derivation performed by Zhang and Prosperetti [1] in their fundamental paper in 1993. This derivation allows us to introduce the notations and some of the issues. It is based on the use of generalized functions which are relatively touchy to manipulate.

Second, we present and shortly discuss the Cahn-Hilliard and Allen-Cahn equations which were built to represent the separation process of two partially miscible fluids and are based on a potential energy argument. We also discuss the usual form given to the surface tension, with a particular emphasis on the usefulness of the conservative form making apparent a possible potential energy origin.

Third, we postulate a momentum equation of a single component fluid, having a constant density but not necessarily occupying all the local volume, introducing the concept of intrinsic volume fraction, that is a volume fraction having sense before any averaging process. This methodology is widely discussed and used in Drew and Passman [2]. The postulated equation is constrained to revert to the normal equation for the single component flow upon summation on the different phases. We discuss the constraints on the different terms of the postulated equation. Special attention is given to the

momentum exchange term.

Fourth, we put in evidence how the energy concept, first encountered for the Cahn-Hilliard equation, can be made apparent in the terms on the momentum equation. In the traditional approach (see Jacqmin [11]), the forces are derived from the potential energies by consideration on the entire system. We restrict this approach to the phases taken separately. The forces are thus derived on a phase basis. As there is no more ambiguity on the velocity field to be used, the forces can be derived in exact math.

Fifth, we arrive to the point. We relate the forces to the difference between the phase velocities through a dynamic equilibrium assumption. The equilibrium assumption is confronted positively with some known features: classical diffusion, gravity and baro-diffusion.

Sixth, the surface tension is considered in this extended framework. We propose an energy defining the surface tension, how it is split between the phases and what is the consequence on the phase transport equations. The choice operated allows to keep the classical Landau [7] term unchanged.

Seventh, we resume the whole picture in the form of a set of proposed equations. And, finally we make a short discussion.

## 2 System of equations for two immiscible fluids

We consider the case of two immiscible fluids A and B occupying different complementary parts of a shared common domain  $\Omega$ . The volume occupied by the fluid A (resp. B) is characterized by the unit value of its support function "a" (resp. "b"). We will also use the subscript "a" (resp. "b") for all and any physical quantity related to fluid A (resp. B). Stating that "a" and "b" are support functions means that they can take only the discrete values 0 and 1. The property that together the two fluids occupy all the available volume is mathematically stated as:

$$a + b = 1 \text{ in } \Omega, \quad (1)$$

The property that the two fluids are immiscible is mathematically stated as:

$$ab = 0 \text{ in } \Omega, \quad (2)$$

The volume occupied by each phase is driven by the evolution of its boundary

$$\partial_t a + u_{\Gamma_a} \cdot \nabla a = 0 \text{ in } \Omega, \quad (3)$$

$$\partial_t b + u_{\Gamma_b} \cdot \nabla b = 0 \text{ in } \Omega, \quad (4)$$

where  $u_{\Gamma_a}$  is the velocity of the boundary of phase A.

We restrict our analysis to cases in which mass exchange can occur only through an existing interface. For example, a bubble of phase A cannot spontaneously appear in the bulk of phase B from nothing. It can however collapse and disappear if care is taken for the dependence of mass exchange with surface curvature. The interface velocity has two components, one is the fluid velocity, the other is related to the local mass transfer rate  $\dot{m}_{ab} = -\dot{m}_{ba}$  between the phases of respective densities  $\rho_a$  and  $\rho_b$ .

$$\partial_t a + \left(u_a - \frac{\dot{m}_{ab}}{\rho_a} n_a\right) \cdot \nabla a = 0 \text{ in } \Omega, \quad (5)$$

$$\partial_t b + \left(u_b - \frac{\dot{m}_{ba}}{\rho_b} n_b\right) \cdot \nabla b = 0 \text{ in } \Omega, \quad (6)$$

where  $n_a$  (resp.  $n_b$ ) is a regular vector field whose trace on the surface  $\Gamma_A$  (resp.  $\Gamma_B$ ) coincide with the surface normal oriented towards the interior of A (resp. B). This convention is opposite to the usual one but allows to have formally  $n_a$  and  $\nabla a$  oriented in the same direction. It also allows to represent  $\nabla a$  as  $n|\nabla a|$ .

From equation (1) one has that

$$\partial_t(a + b) = 0 \text{ in } \Omega, \quad (7)$$

$$\nabla(a + b) = 0 \text{ in } \Omega \quad (8)$$

One should also get easily convinced that  $n_a \cdot \nabla a = n_b \cdot \nabla b$  so that

$$\dot{m}_{ab} n_a \cdot \nabla a + \dot{m}_{ba} n_b \cdot \nabla b = 0, \quad (9)$$

but in general, in presence of mass transfer between fluids of different density, none of  $u_a$ ,  $u_b$  and  $u_{\Gamma_a}$  coincide on the interface. Moreover,  $u_{\Gamma_a}$  and  $u_{\Gamma_b}$  must have only the normal component coinciding on the interface.

Each fluid is supposed to follow the behavior dictated by the Navier-stokes equations. That is:

$$\partial_t(\rho_a u_a) + \nabla \cdot (\rho_a u_a u_a) + \nabla P_a + \nabla \cdot \tau_a = \rho_a g + F_a \text{ in } \Omega_a(t) \quad (10)$$

$$\partial_t(\rho_b u_b) + \nabla \cdot (\rho_b u_b u_b) + \nabla P_b + \nabla \cdot \tau_b = \rho_b g + F_b \text{ in } \Omega_b(t) \quad (11)$$

where  $P_a$  is the phase A pressure,  $\tau_a$  the extra-stress tensor,  $g$  the gravity acceleration and  $F_a$  the resultant of the internal forces, usually null for homogeneous phases, so it will be omitted hereafter. We do not forget the mass conservation equations, degenerating for constant phase density in the divergence free constraints:

$$\partial_t \rho_a + \nabla \cdot (\rho_a u_a) = 0 \text{ in } \Omega_a(t) \quad (12)$$

$$\partial_t \rho_b + \nabla \cdot (\rho_b u_b) = 0 \text{ in } \Omega_b(t) \quad (13)$$

The problem is that the velocities  $u_a$  and  $u_b$  (but also the densities  $\rho_a$  and  $\rho_b$ ) have no physical meaning respectively in domain  $\Omega_b$  and  $\Omega_a$ . But, because we want to write formulas valid in all the domain considered, we must extend  $u_a$  and  $u_b$  to the whole domain. The extension can be arbitrary but we want to be authorized to use the standard derivation rules like  $\nabla \cdot (au_a) = u_a \cdot \nabla a + a \nabla \cdot u_a$  taking into account that  $a$  is a discontinuous function. For this reason, we choose to consider regular extensions of  $u_a$  and  $u_b$ , preserving at least their continuity and the continuity of their divergence. Similarly,  $\rho_a$  and  $\rho_b$  are extended possibly by a constant value all over the domain. Note that we can not extend the divergence free property of  $u_a$  and  $u_b$  to the entire domain when the interface has closed contours because of the the authorized mass exchange. Nevertheless, by continuity, if  $u_a$  and  $u_b$  are divergence-free in their respective domains, they are also divergence free on the interface. We could be however faced with mathematical inconsistency in pathological cases with discrete change in the topology on the interface, such as the disappearance of a bubble or droplet.

The variables can be interpreted either on a phase basis or on a global basis. The relation between them can be made by use of the "a" and "b" variable. The global variables can therefore be expressed in terms of the phase variables as follows.

$$\rho = a\rho_a + b\rho_b \quad (14)$$

$$P = aP_a + bP_b \quad (15)$$

$$u = au_a + bu_b \quad (16)$$

$$\rho u = a\rho_a u_a + b\rho_b u_b \quad (17)$$

$$\rho uu = a\rho_a u_a u_a + b\rho_b u_b u_b \quad (18)$$

These equations simply state that the density is the phase A density when  $a = 1$  and is the phase B density when  $a = 0$ , and so on for pressure, momentum and  $\rho uu$ . Specifically,  $u$  is really the velocity associated to  $\rho$ .

These definitions lead to additional properties that can prove useful for the derivation of the unclosed terms. For example:

$$\rho a = a\rho_a \quad (19)$$

$$\rho ua = a\rho_a u_a \quad (20)$$

$$a = a^2 \quad (21)$$

Moreover, all properties should remain true inverting "a" and "b".

The domain of the single phase Navier-Stokes equations can be extended



to all  $\Omega$  simply by multiplying by the respective support functions.

$$a\partial_t(\rho_a u_a) + a\nabla \cdot (\rho_a u_a u_a) + a\nabla P_a + a\nabla \cdot \tau_a = a\rho_a g \quad \text{in } \Omega \quad (22)$$

$$b\partial_t(\rho_b u_b) + b\nabla \cdot (\rho_b u_b u_b) + b\nabla P_b + b\nabla \cdot \tau_b = b\rho_b g \quad \text{in } \Omega \quad (23)$$

and

$$a\partial_t \rho_a + a\nabla \cdot (\rho_a u_a) = 0 \quad \text{in } \Omega \quad (24)$$

$$b\partial_t \rho_b + b\nabla \cdot (\rho_b u_b) = 0 \quad \text{in } \Omega \quad (25)$$

Turning back to the volume equations (5) and (6), multiplying by the respective density, we obtain the single phase density equations. It comes:

$$\rho_a \partial_t a + \rho_a u_a \cdot \nabla a = \dot{m}_{ab} n_a \cdot \nabla a \quad (26)$$

$$\rho_b \partial_t b + \rho_b u_b \cdot \nabla b = \dot{m}_{ba} n_b \cdot \nabla b \quad (27)$$

Summing the volume conservation equations and the mass conservation equations extended to the entire domain, we get the conservative form of the volume fraction equations:

$$\partial_t(\rho_a a) + \nabla \cdot (a \rho_a u_a) = \dot{m}_{ab} n_a \cdot \nabla a \quad (28)$$

$$\partial_t(\rho_b b) + \nabla \cdot (b \rho_b u_b) = \dot{m}_{ba} n_b \cdot \nabla b \quad (29)$$

Summing these two equations, we recognize the global mass conservation term. That is:

$$\partial_t \rho + \nabla \cdot (\rho u) = 0, \quad (30)$$

which is quite comforting.

To simplify the notation, we define the phase source term as:

$$\dot{S} = \dot{m}_{ab} n_a \cdot \nabla a \quad (31)$$

Therefore:

$$\partial_t(\rho_a a) + \nabla \cdot (a \rho_a u_a) = \dot{S} \quad (32)$$

$$\partial_t(\rho_b b) + \nabla \cdot (b \rho_b u_b) = -\dot{S} \quad (33)$$

The term  $\dot{S}$  is here a scalar distribution with support on the interface. However equations 32 and 33 are valid even for variable distributions of the volume fractions. We introduce the notation:  $\delta \frac{1}{\rho} = \frac{1}{\rho_b} - \frac{1}{\rho_a}$ . Summing the original volume equations, we get a new time independent equation:

$$(u_a - u_b) \cdot \nabla a = \delta \frac{1}{\rho} \dot{S}, \quad (34)$$

equivalent to

$$\nabla \cdot u - [a\nabla \cdot u_a + b\nabla \cdot u_b] = \delta \frac{1}{\rho} \dot{S}, \quad (35)$$

or, using the incompressibility of each separated flow, if applicable:

$$\nabla \cdot u = \delta \frac{1}{\rho} \dot{S}. \quad (36)$$

Note that for the first time, we have broken the symmetry of representation.

Operating in a similar way, we will show how the global momentum equation can be retrieved from the momentum equation of both phases. Now, we incorporate the multipliers under the differential operators in equations 10,11 to get:

$$\begin{aligned} \partial_t(a\rho_a u_a) + \nabla \cdot (a\rho_a u_a u_a) + \nabla(aP_a) + \nabla \cdot (a\tau_a) &= a\rho_a g \\ &+ (\rho_a u_a) \partial_t a + (\rho_a u_a u_a) \cdot \nabla a + P_a \nabla a + \tau_a \cdot \nabla a \end{aligned} \quad (37)$$

$$\begin{aligned} \partial_t(b\rho_b u_b) + \nabla \cdot (b\rho_b u_b u_b) + \nabla(bP_b) + \nabla \cdot (b\tau_b) &= b\rho_b g \\ &+ (\rho_b u_b) \partial_t b + (\rho_b u_b u_b) \cdot \nabla b + P_b \nabla b + \tau_b \cdot \nabla b \end{aligned} \quad (38)$$

or, substituting with the progress and regress variable equations multiplied respectively by  $u_a$  and  $u_b$ :

$$\begin{aligned} \partial_t(a\rho_a u_a) + \nabla \cdot (a\rho_a u_a u_a) + \nabla(aP_a) + \nabla \cdot (a\tau_a) &= a\rho_a g + \\ &u_a \cdot \dot{S} + P_a \nabla a + \tau_a \cdot \nabla a \end{aligned} \quad (39)$$

$$\begin{aligned} \partial_t(b\rho_b u_b) + \nabla \cdot (b\rho_b u_b u_b) + \nabla(bP_b) + \nabla \cdot (b\tau_b) &= b\rho_b g \\ &- u_b \cdot \dot{S} + P_b \nabla b + \tau_b \cdot \nabla b \end{aligned} \quad (40)$$

Direct averaging of these equations may lead to the Eulerian two-phase flow approach. Summing these two equations, we recognize on the left hand side the momentum equation for the global variables:

$$\begin{aligned} \partial_t(\rho u) + \nabla \cdot (\rho u u) + \nabla P &+ \nabla \cdot \tau = \rho g + (u_a - u_b) \cdot \dot{S} \\ &+ (P_a - P_b) \nabla c + (\tau_a - \tau_b) \cdot \nabla c \end{aligned} \quad (41)$$

that is:

$$\partial_t(\rho u) + \nabla \cdot (\rho u u) + \nabla P + \nabla \cdot \tau = \rho g + F \quad (42)$$

and

$$F = (u_a - u_b) \cdot \dot{S} + (P_a - P_b) \nabla a + (\tau_a - \tau_b) \cdot \nabla a. \quad (43)$$

It means that the interpretation of a two-phases reactive flow as a unique flow leads to the appearance of a force term in the momentum equation localized on

the interface. We will show that this force vanishes if we make the necessary hypothesis that the impulse and  $\tau$  are continuous across the interface, in a reference frame linked to the interface. If we assume that  $\tau$  is continuous across the frontier then the former equation simplifies to:

$$F = (u_a - u_b) \cdot \dot{S} + (P_a - P_b) \nabla a. \quad (44)$$

To keep invariance properties, we can assume that the tangential velocity is continuous across the interface. Therefore, using equation 34:

$$(u_a - u_b) = \delta \frac{1}{\rho} m_{ab} \cdot n_a \quad (45)$$

so that

$$(u_a - u_b) \cdot \dot{S} = \delta \frac{1}{\rho} \dot{m}_{ab}^2 \cdot \nabla a \quad (46)$$

The pressure drop can be estimated considering that the total impulse is conserved through the interface in a reference frame linked to the interface. Considering that the interface velocity is  $u_a - \frac{\dot{m}_{ab}}{\rho_a} \cdot n_a$ , or equivalently  $u_b - \frac{\dot{m}_{ba}}{\rho_b} \cdot n_b$  we have:

$$P_a + \rho_a [u_a - (u_a - \frac{\dot{m}_{ab}}{\rho_a} \cdot n_a)]^2 = P_b + \rho_b [u_b - (u_b - \frac{\dot{m}_{ba}}{\rho_b} \cdot n_b)]^2 \quad (47)$$

$$P_a - P_b = \rho_a [\frac{\dot{m}_{ab}}{\rho_a}]^2 - \rho_b [\frac{\dot{m}_{ba}}{\rho_b}]^2 \quad (48)$$

leading to:

$$P_a - P_b = \dot{m}_{ab}^2 \delta \frac{1}{\rho} \quad (49)$$

Combining this result with 46, then  $F = 0$ , that is:

$$\partial_t(\rho u) + \nabla \cdot (\rho u u) + \nabla P + \nabla \cdot \tau = \rho g. \quad (50)$$

In presence of a surface tension  $\sigma$  when at least one of the phases is liquid, the pressure difference is incremented by  $\sigma(\nabla \cdot n_a)$  and  $F = -\sigma(\nabla \cdot n_a) \nabla a + < n_a, \nabla a > \nabla_S \sigma$ , where  $\nabla_S$  is the surface gradient. It should be noted that the surface tension does not appear in the single phase equations but only in the global one, defining an interface condition. It is also normal that the surface tension could not be completely directly derived from the single phase equations because the mere existence and the intensity of the surface tension is independent from the physical quantities present in the single phase equations. In other words, given the physical properties necessary to write their respective Navier-stokes equations, we can decide independently if they will be miscible or immiscible.

From both momentum equations and the impulse equation, we have derived only one global equation. So, it seems that we have lost some information. For immiscible fluids, this is not the case. In effect, velocity and pressure of each phase is perfectly known from the global velocity and pressure and from the volume fraction equation. This is no more the case when the phases are allowed to mix because the values given by the global equation cannot anymore easily be specialized to the separate phases.

### 3 On surface tension and immiscibility

We start with some empirical qualitative consideration. Surface tension is an intrinsic property of a medium pair. It appears only when at least one of the media is a liquid. Surface tension is also defined for a solid. It is used to determine the angle formed by two immiscible fluids on a wall. It is also strongly linked with the concept of wettability. Here, we want to deal only with two immiscible fluids. So, at least one of them is liquid, because gases are always miscible. What is strange at first glance is that liquids can continuously change to gas on a temperature/pressure diagram if they "travel" around the triple point. So, there is a continuous transformation of most, if not all, fluid pairs from immiscibility characterized by a positive surface tension coefficient to miscibility characterized by a positive diffusion coefficient. The problem is that the surface tension is present in the momentum equation while the diffusion coefficient is in the mass fraction equation. But both should be representative of the same physico-chemical property. We would like to find a unified representation of the phenomena, at least for simple cases.

#### 3.1 Cahn-Hilliard equation

One tentative to represent the behaviour of two immiscible fluids has led to the famous Cahn-Hilliard equation. The Cahn-Hilliard equation describes the evolution of a conserved concentration field during phase separation<sup>3</sup>. One of its simplest isotropic version is given below:

$$\partial_t c = \alpha \Delta[(1 - 2c)c(1 - c)] - \beta \Delta^2 c. \quad (51)$$

where  $\alpha$  and  $\beta$  are positive parameters and  $c$  has the same meaning of our "a" or "b". The equation comes from an energy whose density is  $e = \frac{\alpha}{2}c^2(1 - c)^2 + \frac{\beta}{2}|\nabla c|^2$  and its fastest minimization in the  $L^2$  norm. The first term in the RHS is a second order contracting term, while the second one is a fourth order diffusing term. Given a representative length  $\lambda$ , of the region

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<sup>3</sup><http://www.ctcms.nist.gov/wcraig/variational/node9.html>

of intermediary values of  $c$  (i.e. the diffuse interface length), the first RHS term scales like  $\lambda^{-2}$  while the second one like  $\lambda^{-4}$ . Therefore for large  $\lambda$ , the contracting term dominates while for small  $\lambda$  the diffusing term dominates. That is, a wide interface will tend to contract while a thin one will tend to dilate. The equilibrium is obtained when  $\lambda^2$  is order  $\beta/\alpha$ .

For our initial concern, the derivation of a naturally contracting system of equation, such that the interface length is no more than one or two computational cells, the fourth order equation is out of range. In effect, the discretisation of a fourth order operator requires (in 1D) to take information up to a distance of two cells in both direction (for usual finite volumes). This is incompatible with the maximum two-cells interface objective. It is also not possible to just set  $\beta = 0$  because the strength of the contracting term would result unbounded for arbitrary small discretisation.

However, the idea that phase separation, for which surface tension is the final residual trace, must be based on energy considerations is very attractive.

### 3.2 Allen-Cahn equation

The technical burden associated with the Cahn-Hilliard equation fourth order term has been widely recognized, see for example Yang et al.[3]. The result is that many authors have chosen to represent the same physical phenomena with a simpler (lower order) equation, the Allen-Cahn equation, derived for the same reason. Its simplest form is:

$$\partial_t c = -\alpha(1 - 2c)c(1 - c) + \beta\Delta c \quad (52)$$

this time, the diffusive term is the classical Laplacian operator, scaling like  $\lambda^{-2}$  while the contracting term is scalar and scales like  $\lambda^0$  with the equilibrium still obtained when  $\lambda^2$  is order  $\beta/\alpha$ .

The equation arises from the fastest minimization of the previous energy, however with regard to a different norm. This equation is much more convenient and has also been studied and simulated in a huge number of papers. While the order of the equation is convenient, it is straightforward to see that the equation is non-conservative. This defect has been recognized and has generally been corrected by use of a non local Lagrange multiplier:

$$\partial_t c = -\alpha(1 - 2c)c(1 - c) + \beta\Delta c + \epsilon(t). \quad (53)$$

Unfortunately, this solution is completely unfit for multi-purpose CFD codes. In effect, the Lagrange multiplier is simply redistributing mass (a small quantity everywhere) slightly dirtying all the spatial field, just to comply with the overall mass preservation. In the CFD context, people usually consider

the local mass preservation as a "non negotiable" property. By the way, only the scalar term is not conservative and it would be very convenient to find out a similar one (with regards to the scaling in  $\lambda$ ) which would be conservative.

Both equations are constructed on the same scheme. Evolution of the concentration arises from the balance of two contributions, a linear higher order diffusive one impeding the degeneracy due to a non-linear lower order contracting one. In the Cahn-Hilliard equation, one cannot just set  $\beta = 0$  because only a Laplacian with a "negative" diffusivity is left, and a phase separation leads to an unbounded energy of the surface. This feature is not true setting the coefficient  $\beta$  to zero in the Allen-Cahn equation. In this case, the concentration simply decays to zero or one depending whether the initial value is greater or lower than one half. We can also see that in this case, most of the physico-chemical process tentatively modelled is lost. However, we think that this loss of physical meaning is simply caused by the absence of local mass conservation. So, we will try to derive a conservative term, however scaling with a power of  $\lambda$  more than minus one for small  $\lambda$ , so that its integral effect will vanish in the limit of a discontinuous interface.

### 3.3 Representation of the surface tension

The classical representation of the surface tension is, as already written:

$$F = -\sigma(\nabla \cdot n_a)\nabla a + |\nabla a|\nabla_S \sigma \quad (54)$$

with  $\sigma$  the surface tension coefficient,  $\nabla_S = (\delta_{ij} - n_i n_j)\partial_j$  is the surface gradient and  $|\nabla a|$  is a clear notation abuse that we will use hereinafter for  $\langle \nabla a, n_a \rangle$ . The formula above is valid only if the condition  $\nabla n^2 = 0$  holds on the interface. That is, if the field  $n$  coinciding with the unit normal on the interface is prolonged to a unit field out of the interface, at least at the first order (the slope of the normal module must be zero on the interface). Otherwise, the term  $\nabla \cdot n_a$  has to be changed to  $\nabla_S \cdot n_a$ .

The form of the surface tension is rather specific. It cannot be put under gradient form, but it may be represented, as found out by several authors [4, 5] under a divergential form, as follows:

$$F = \nabla \cdot T \quad (55)$$

$$T = \sigma|\nabla a|(\delta_{ij} - n_i n_j). \quad (56)$$

Using the identity matrix  $I$ , we have:

$$T = G(I - nn) \quad (57)$$

$$G = \sigma|\nabla a| \quad (58)$$

This formula outlines the natural potential  $G$  constitutive of the surface tension.

A point which is worth remarking is that whatever monotonous derivable function  $\Phi$  of "a" such that  $|\Phi(1) - \Phi(0)| = 1$  can be used for the definition of  $F$  instead of "a".

For example, taking  $\Phi = \frac{\rho^2}{\rho_a^2 - \rho_b^2}$ , we have  $\nabla\Phi = \frac{2\rho}{\rho_a + \rho_b} \nabla a$  and

$$T = \rho \frac{2\sigma}{\rho_a + \rho_b} |\nabla a| (\delta_{ij} - n_i n_j), \quad (59)$$

that is a potential part plus a convective transport with velocity modulus  $V = \sqrt{\frac{2\sigma}{\rho_a + \rho_b} |\nabla a|}$ , if we manage to give some meaning to this velocity for arbitrary small interface.

This choice of  $\Phi$ , making the density appear has already been made in the reference work of Brackbill and al. [6]. They noticed that doing this, the interface width was better conserved. However, one would expect less discretisation error by considering directly  $\nabla\Phi$  and not its expansion. This leads in turn to consider the square of the density as a fundamental parameter which is a rather unusual choice.

### 3.4 Derivation of the surface tension from energy consideration

The derivation of the classical form of the surface tension is given in Landau [7]. Here we derive it again on an energy argument.

Let us postulate a "free" energy  $G$  to be globally minimized by the flow in the form:

$$G = \int_{\Omega} \sigma |\nabla a| \quad (60)$$

We want to know how is evolving  $G$  in time if the material  $A$  is displaced by a velocity field "v" (vanishing on the domain boundary). Being a conserved quantity, the volume fraction time evolution is locally given by:

$$\partial_t a + \nabla \cdot (av) = 0. \quad (61)$$

The surface tension coefficient  $\sigma$  is not likely to be a conserved quantity, but is a local property of the volume fraction, for example depending mainly on temperature. In a first approximation, we consider that  $\sigma$  is convected by the flow:

$$\partial_t \sigma + v \cdot \nabla \sigma = 0. \quad (62)$$

The generalized force aimed at minimizing the potential  $G$  is given by  $F = -\nabla G$  according to the formula:

$$d_t G_v = \langle \nabla G, v \rangle_{L^2(\Omega)} \quad (63)$$

with the scalar product on the right hand side classically defined in our case as:

$$\langle f, g \rangle_{L^2(\Omega)} = \int_{\Omega} f g. \quad (64)$$

We just have therefore to evaluate,  $d_t G_v$  and represent it, if feasible, under the form  $\langle -F, v \rangle_{L^2(\Omega)}$ .

The domain of evaluation  $\Omega$  does not change in time and we can write:

$$d_t G_v = \int_{\Omega} \partial_t (\sigma |\nabla a|) \quad (65)$$

$$= \int_{\Omega} \sigma \partial_t |\nabla a| + |\nabla a| \partial_t \sigma \quad (66)$$

Only the term  $\partial_t |\nabla a|$  may not be considered trivial so we evaluate it separately, using the derivation chain rule:

$$\partial_t |\nabla a| = \partial_t \langle \nabla a, \nabla a \rangle^{\frac{1}{2}} \quad (67)$$

$$= \langle \nabla a, \nabla a \rangle^{-\frac{1}{2}} \langle \nabla a, \partial_t \nabla a \rangle \quad (68)$$

$$= n \cdot \nabla \partial_t a \quad (69)$$

$$= -n \nabla [\nabla \cdot a v] \quad (70)$$

so that

$$\begin{aligned} d_t G_v &= - \int_{\Omega} \sigma n \nabla [\nabla \cdot a v] + |\nabla a| v \cdot \nabla \sigma \\ &= \int_{\Omega} \nabla \cdot (\sigma n) (v \cdot \nabla a + a \nabla \cdot v) - |\nabla a| v \cdot \nabla \sigma \\ &= \langle \nabla \cdot (\sigma n) \nabla a - |\nabla a| \nabla \sigma, v \rangle_{L^2(\Omega)} + \int_{\Omega} (\nabla \cdot \sigma n) a \nabla \cdot v \\ &= \langle \sigma \nabla \cdot n \nabla a - |\nabla a| \nabla_S \sigma, v \rangle_{L^2(\Omega)} + \int_{\Omega} (\nabla \cdot \sigma n) a \nabla \cdot v. \end{aligned} \quad (71)$$

and the classical formulation is retrieved on the condition that  $a \nabla \cdot v = 0$ . This means that we force the velocity field to be divergence free everywhere the volume fraction is non zero. Typically this allows a bubbly flow in which the bubbles can shrink under pressure. The condition is quite reasonable when phase A is liquid, and the surface tension is therefore considered a property of the phase A.

Because the condition that  $a \nabla \cdot v = 0$  is a priori not satisfied with fluids allowed to present some partial mixing, some additional work must be done to



extend properly the expression of surface tension. Managing in this context to preserve the expression of the surface tension and its link with an energy functional would be greatly appreciated. To reach this objective, we will need first to extend all the former construction of the Navier-stokes equation to mixing phases.

## 4 System of equations for two miscible fluids

In the first part of this document, we have derived the global Navier-stokes equations for density and momentum from the single phases equations in the limiting case of two immiscible phases. While the derivation can be made quite rigorous, the surface tension cannot be derived in this way but comes as an external consideration. To be naturally inserted in the final equation, the surface tension should be in some way included in the single phase equations. Looking at the Cahn-Hilliard and Allen-Cahn equations, we have seen that the surface tension can be interpreted as the terminal state of a phase separation process. However, these equations do not allow the phase separation to arrive at completion, having a small but non null asymptotic interface width. And unfortunately, degenerating the equations for zero asymptotic width leads to loss of physical meaning. What remains crucial in this approach is the energetic consideration: the interface sharpens and reduces because doing this the fluid minimizes its energy. In the global momentum equation, this energy consideration should naturally appear as minus the generalized gradient of this energy.

By setting the energy to be precisely  $G = \int_{\Omega} \sigma |\nabla a|$ , we have retrieved the classical form of the surface tension, under the condition that no active mixing or phase separation is allowed. This is a start, as it gives an asymptotic limit to be respected. The problem lies in a good general mathematical definition of the local measure of an interface. Taking it to be  $|\nabla a|$  is extremely convenient, except for one small defect: smearing a regular (flat) interface do not increase (and do not decrease, fortunately) the energy  $G$ . Smearing is neutral with regard to the energy, so that minimizing the energy does not affect interface smearing. As in absence of surface tension, thermal agitation induces phase mixing, surface tension should be responsible for suppressing this effect. The free energy  $G$  must be such that it decisively operates to counteract interface smearing.

By postulating single phase equations in which mixing is allowed, we could insert the additional energy term which would be active where mixing is ef-

fective. This is what we do now. We postulate a general form of the single phases momentum equations and try to eliminate the unknown terms by considerations on the overall momentum equation.

We should note that this idea of postulating the single phase equation is not new and has already been developed by several authors, see for example Boyer [8]. Differences between the postulated equations are normally small but existing. They depend widely on the specific scope of the research.

## 4.1 Momentum equation

Here we consider two gaseous phases correctly described at the molecular level with a rigid sphere model.

When considering separately the momentum equation of a single phase in a mixture, the main change is that the integral collision term in the Boltzmann equation and the related Enskog theory does not cancel any more and results in a term of exchange with the other phase, see [9]. This leads to postulate the single phase equations in the form:

$$\partial_t(a\rho_a u_a) + \nabla \cdot (a\rho_a u_a u_a) + \nabla \cdot \mathbb{P}_a - \nabla \cdot a\mu\Pi u = I_{ab} + a\rho_a g + F_a \quad (72)$$

$$\partial_t(b\rho_b u_b) + \nabla \cdot (b\rho_b u_b u_b) + \nabla \cdot \mathbb{P}_b - \nabla \cdot b\mu\Pi u = I_{ba} + b\rho_b g + F_b \quad (73)$$

with the momentum exchange term  $I$  satisfying  $I_{ab} + I_{ba} = 0$ .

One tends to postulate a phase pressure term (isotropic part) in the form  $a\nabla P$  rather than  $\nabla aP$ . The difference  $P\nabla a$  can be put in the yet undecided force  $F_a$ , the sum of the differences being zero. The same argument can be used for the extra-stress term.

With this foreword in mind, we now discuss the pressure terms. We have used the single phase pressure tensors  $\mathbb{P}_a$  and  $\mathbb{P}_b$  which are connected with the quadratic deviation from some “mean” velocity. This mean velocity could be the single phase mean velocity or the mixture mean velocity. The tensor representation changes accordingly.

$$\mathbb{P}_{u_a} = \frac{a\rho_a \overline{(u'_a - u_a)(u'_a - u_a)}}{\quad} \quad (74)$$

$$\mathbb{P}_{u_a} = \frac{a\rho_a \overline{(u'_a - u + u - u_a)(u'_a - u + u - u_a)}}{\quad} \quad (75)$$

$$\begin{aligned} \mathbb{P}_{u_a} &= a\rho_a [\overline{(u'_a - u)(u'_a - u)} + (u - u_a)(u - u_a) - u(u - u_a) - (u - u_a)u] \\ \mathbb{P}_{u_a} &= \mathbb{P}_{a,u} + a\rho_a(u_a u_a - uu) \end{aligned} \quad (76)$$

and similarly

$$\mathbb{P}_{u_b} = \mathbb{P}_{b,u} + b\rho_b(u_b u_b - uu) \quad (77)$$

where  $\mathbb{P}_{a,u}$  and  $\mathbb{P}_{b,u}$  are partial pressure tensors referred to the mean mass weighted velocity  $u$  defined by:

$$u = a\rho_a u_a + b\rho_b u_b. \quad (78)$$

This means that the partial pressure tensors are potentially unitary in at most one referential system.

Summing the partial pressures, we have:

$$\mathbb{P}_{u_a} + \mathbb{P}_{u_b} = \mathbb{P}_{a,u} + \mathbb{P}_{b,u} + a\rho_a u_a u_a + b\rho_b u_b u_b - \rho w u \quad (79)$$

and according to the formula

$$\rho w u = a\rho_a u_a u_a + b\rho_b u_b u_b - \frac{ab\rho_a \rho_b}{\rho} (u_b - u_a)(u_b - u_a) \quad (80)$$

we have

$$\mathbb{P}_{u_a} + \mathbb{P}_{u_b} = \mathbb{P}_{a,u} + \mathbb{P}_{b,u} + \frac{ab\rho_a \rho_b}{\rho} (u_b - u_a)(u_b - u_a) \quad (81)$$

This means that the sum of the partial pressures does change if they refer to their own local velocities or to mass averaged one.

Defining  $F = F_a + F_b$ , the sum of the non gravity forces acting separately on the single phases, we now can sum the two phase momentum equations to get:

$$\begin{aligned} \partial_t(\rho u) + \nabla \cdot (\rho u u) + \nabla \cdot [\mathbb{P}_a + \mathbb{P}_b + \frac{ab\rho_a \rho_b}{\rho} (u_b - u_a)(u_b - u_a)] \\ = \nabla \cdot \mu \Pi u + \rho g + F. \end{aligned} \quad (82)$$

We are thus induced to choose  $\mathbb{P}_a = \mathbb{P}_{a,u}$  and  $\mathbb{P}_b = \mathbb{P}_{b,u}$ , so that the equation simplifies to:

$$\partial_t(\rho u) + \nabla \cdot (\rho u u) + \nabla \cdot [\mathbb{P}_{u_a} + \mathbb{P}_{u_b}] = \nabla \cdot \mu \Pi u + \rho g + F. \quad (83)$$

It is therefore very tempting that even for simple cases without surface tension, the pressure tensors of the single phases are unitary only in their own natural referential, at least if we want the postulated equations to hold.

To get back to the usual momentum equation, we can relate the partial pressure tensors to the mean mass weighted velocity and choose it unitary in this referential. If we take:

$$\mathbb{P}_a = aPI - a\rho_a(u_a u_a - u u) \quad (84)$$

$$\mathbb{P}_b = bPI - b\rho_b(u_a u_b - u u) \quad (85)$$

then

$$\mathbb{P}_a + \mathbb{P}_b = PI - \frac{1}{\rho} ab\rho_a \rho_b (u_b - u_a)(u_b - u_a) \quad (86)$$

$$\mathbb{P}_{u_a} + \mathbb{P}_{u_b} = PI \quad (87)$$

and we retrieve the usual momentum equation in its original form.

$$\partial_t(\rho u) + \nabla \cdot (\rho u u) + \nabla P + \nabla \cdot \mu \Pi u = \rho g + F. \quad (88)$$

The problem with this choice of partial pressures is that the single phase momentum equation revert a totally unsatisfactory shape. In effect, the convective transport of the phase velocity simply disappears:

$$\partial_t(a\rho_a u_a) + \nabla \cdot (a\rho_a u u) + \nabla \cdot aP - \nabla \cdot a\mu\Pi u = I_{ab} + a\rho_a g + F_a \quad (89)$$

This illustrate the devastating influence of the hypothesis made on the pressure and its splitting among the phases.

On the other hand, if the phase pressure are unitary in their own system of reference, the momentum equation inherit of the additional term:  $\nabla \cdot \frac{ab\rho_a\rho_b}{\rho}(u_b - u_a)(u_b - u_a)$ , that we would prefer to avoid. Things get even worse if we test a referential linked to the apparent velocity  $v = au_a + bu_b$ .

We thus make a step back and reconsider the postulated phase momentum equations. Looking at a quite general representation of the conservation equations, for a property  $X_a$  of phase A, we can observe a conservation equation of the form:

$$\partial_t(\rho_a X_a) + \nabla \cdot (\rho_a u X_a) + \nabla \cdot \Phi_a = S_a + I_a \quad (90)$$

- $\nabla \cdot \rho_a u X_a$  is the "approximate" convective flux (main flux),
- $\nabla \cdot \Phi_a$  is a corrective flux (deviation),
- $S_a$  is the source of  $\rho_a X_a$  (there may be more than one),
- $I_a$  is a term of exchange with the other phase.

In this representation, the flux is split into two parts, an approximate first one, the convective flux, and a correction. The correction is subject to intense modelling. We must stress the fact that the main flux is driven by the mass fraction velocity and not by the phase velocity.

Application to the phase momentum leads to:

$$\partial_t a\rho_a u_a + \nabla \cdot a\rho_a u u_a + \nabla \cdot a([P + P_0]I + \tau) = a\rho_a g + F'_a + I_a \quad (91)$$

$$\partial_t b\rho_b u_b + \nabla \cdot b\rho_b u u_b + \nabla \cdot b([P + P_0]I + \tau) = b\rho_b g + F'_b + I_b, \quad (92)$$

where  $g$  is the gravity acceleration,  $P_0$  is the spatially constant time dependant part of the pressure,  $I$  the identity matrix, while  $F'_a$  and  $F'_b$  contribute to diffusion or phase separation and surface tension effects.

Summing the two phase momentum equations gives back the classical momentum NSE under the conditions:

- $I_a + I_b = 0$ , as we expect from exchange terms
- $F'_a + F'_b = F$ .

To simplify the representation, we split the corrective flux term:

$$\nabla \cdot a([P + P_0]I + \tau) = a\nabla P + (P + P_0)\nabla a + \tau\nabla a + a\nabla \cdot \tau. \quad (93)$$

We can recognize the pressure force in the first term. The second and third terms are related to gradient diffusion and are therefore coupled with  $F'_a$ . Taking  $F_a = F'_a - (P + P_0)\nabla a - \tau\nabla a$ , we have our almost final phase momentum equations:

$$\partial_t a \rho_a u_a + \nabla \cdot a \rho_a u u_a + a \nabla P + a \nabla \cdot \tau = a \rho_a g + F_a + I_a \quad (94)$$

$$\partial_t b \rho_b u_b + \nabla \cdot b \rho_b u u_b + b \nabla P + b \nabla \cdot \tau = b \rho_b g + F_b + I_b, \quad (95)$$

with

- $I_a + I_b = 0$ ,
- $F_a + F_b = F$ .

With this approach, we consider the pressure gradient as a projection of the momentum equation on the field of admissible functions. More precisely, the pressure term is here to ensure that the equation of state is satisfied. For incompressible flows, the equation of states reverts to the condition that the volume velocity  $v = au_a + bu_b$  is divergence free. That is:

$$\nabla \cdot v = 0. \quad (96)$$

With this interpretation, the coincidence of the pressure with the thermodynamic pressure is likely to be lost. There is however a priori a large spectrum of possibility on how to split the projection between the two phase momentum equations. Here, we have the correction applied to the momentum equation proportionally to the volume fraction. In this representation, all the terms depending on the concentration gradient are embedded in  $F_a$  and  $F_b$ , including the term  $P\nabla a$ . This is one of the simplest non trivial form leading to the classical Navier-Stokes equation by direct summation.

$$\partial_t(\rho u) + \nabla \cdot (\rho u u) + \nabla P + \nabla \cdot \tau = \rho g + F. \quad (97)$$

where  $F = F_a + F_b$  is left for the surface tension and any other force.

There is clearly some arbitrariness in the representation. We have chosen the conservative version of the equations with the mass averaged main transport velocity. With either the non-conservative form or with a main transport by the apparent velocity  $v$ , we however do not manage to get back the standard form of NSE. Some parasite term always appear.

## 4.2 Inter-phase momentum transfer

In the single phase momentum equation, there is an exchange term representing the resistance provoked by the mere presence of the other phase. A very crude estimation of this force can be done in this way. We suppose that the force is related to the frequency of elastic collisions between particles of different species moving at their mean velocity. The momentum exchanged is proportional to the momentum relatively to the center of mass of the particle pair  $u_c = \frac{\rho_a u_a + \rho_b u_b}{\rho_a + \rho_b}$ , that is, proportional to  $\rho_a(u_a - u - c) = \frac{\rho_a \rho_b (u_a - u_b)}{\rho_a + \rho_b}$ . All other things being equal, the frequency of collision should be proportional to the number density of particle (i.e. to the volume fraction) of one phase when this number is very small. The simplest way to get this property is to get the frequency of collision proportional to the product of the volume fractions. Finally, the exchange term of phase A is expected to have the form:

$$I_{ab} = Rab(u_b - u_a). \quad (98)$$

This form is not original and is effectively used for example in Boyer [8]. The term  $R$  is a characteristic of the hydraulic resistance of the mixture. Generally speaking,  $R$  could be a tensor, but for an isotropic medium, we expect  $R$  to be a scalar. It is a priori essentially independent of the volume fraction, but it can be made dependent on the volume fraction gradient. We can foresee the coefficient  $R$  in the form:

$$R = R_0(1 + |L\nabla H(a)|^2) \quad (99)$$

where  $L$  is a characteristic length likely to be related to the interface width of multi-phase flow exhibiting some surface tension. For small concentration gradient, such an  $R$  is constant at the first order and we are consistent with the assumption made by Landau to derive the corrective flux. The monotonous normalized function  $H$  is not necessarily related to the one used for the surface tension. It is considered only for the scope of generality but we should consider only the identity function. The power two in the gradient is for convenience. When combined with a contracting term proportional to the first power of the volume fraction gradient, the asymptotic solution will be a wide-less interface reached in infinite time at exponentially decaying velocity.

Last but not least, the coefficient  $R$  of the resistance force could be made anisotropic so as to be larger in the direction  $n$  than in direction  $-n$  to take into account a saturation effect making the concentration bounded between zero and one. For infinite gradients, the resistance to further contraction should also become infinite. We can take:

$$R = R_0(1 + 0.5(1 + \langle n, n_u \rangle |L\nabla a|^2)). \quad (100)$$

We should not need however to go to such precise behaviour for our current purpose.

In turn,  $R_0$  is also the ratio between a density and a time. For consistency, the density is the center of mass density  $\rho_{ab} = \frac{\rho_a \rho_b}{\rho_a + \rho_b}$ . The time is related to the characteristic time scale of the phenomena.

$$R_0 = \frac{1}{\tau} \frac{\rho_a \rho_b}{\rho_a + \rho_b} \quad (101)$$

The time scale thus depends on the phenomena to be controlled. For a control at the molecular level, the time scale should be related to the collision frequency. For a control at the turbulence scale level, the time scale should be related to the turbulence time scale. For a control of numerics, it should be related to the computational time step and the CFL.

### 4.3 Volume fraction equation

The volume fraction equations, when written in conservative form, remain valid for non discrete configurations:

$$\partial_t(\rho_a a) + \nabla \cdot (a \rho_a u_a) = \dot{S} \quad (102)$$

$$\partial_t(\rho_b b) + \nabla \cdot (b \rho_b u_b) = -\dot{S} \quad (103)$$

What we have to do is to relate each phase velocity to the global velocity and to the phase velocity difference:

$$u_a = u - \frac{b \rho_b}{\rho} (u_b - u_a) \quad (104)$$

$$u_b = u + \frac{a \rho_a}{\rho} (u_b - u_a) \quad (105)$$

so that

$$\partial_t(\rho_a a) + \nabla \cdot (a \rho_a u) - \nabla \cdot \left[ \frac{ab \rho_a \rho_b}{\rho} (u_b - u_a) \right] = \dot{S} \quad (106)$$

$$\partial_t(\rho_b b) + \nabla \cdot (b \rho_b u) + \nabla \cdot \left[ \frac{ab \rho_a \rho_b}{\rho} (u_b - u_a) \right] = -\dot{S} \quad (107)$$

if the drift velocity  $u_b - u_a$  is oriented along the concentration gradient. then the equation is diffusive while if it is oriented opposite to the concentration gradient, then the equation is contracting.

From now on, we suppose the phase densities constant. Dividing equations (106) and (107) by their respective density and summing, we get the velocity divergence. What we have to do is to relate each phase velocity to the global velocity and to the phase velocity difference:

$$\nabla \cdot u = \nabla \cdot \left[ (\rho_b - \rho_a) \frac{ab}{\rho} (u_b - u_a) \right] + \delta \frac{1}{\rho} \dot{S} \quad (108)$$

and in absence of source term, the velocity  $v$  defined by:

$$v = u - (\rho_b - \rho_a) \frac{ab}{\rho} (u_b - u_a) \quad (109)$$

is divergence-free.

Rewriting in this case the volume fraction equation in term of  $v$ , we get:

$$\partial_t a + \nabla \cdot (av) - \nabla \cdot [ab(u_b - u_a)] = 0, \quad (110)$$

$$\partial_t b + \nabla \cdot (bv) - \nabla \cdot [ab(u_a - u_b)] = 0. \quad (111)$$

Thus, phase A is convected by the velocity  $u_a = v - b(u_b - u_a)$  and phase B by the velocity  $u_b = v - a(u_a - u_b)$ , such that  $v = au_a + bu_b$  is in fact the divergence-free volume based velocity. This last formulation is adapted for algorithms which consider the volume fraction, such as the VOF algorithm in Starccm+.

It has to be noted that the correction flux  $ab(u_b - u_a)$  is proportional to the phase momentum exchange term. This feature will be critically used in the further derivations.

## 5 Energy consideration

In this section, we try to relate forces and fluxes to energies. By observing the known energies and fluxes, we would like to find rules to be applied to the surface tension. The methodology used here is apparently very common and is based on the conservation of the energy of a system. As explained in Jacqmin [11], if the total energy is conserved, then the change in kinetic energy is minus the change in potential energy. In turn, the rate of change of the kinetic energy is equal, according to Newton's law, to the integral of product velocity times force. Using the arbitrariness of the velocity field, we can thus determine the force derived from a potential energy. There is a hidden flaw in this reasoning when the system is composed of two species of different specific volume. In effect, for a given force, the acceleration of particles of different weight is the same only when the force is proportional to the weight, which, with the exception of gravity, is not true in general.

The concept can however be applied to a sub-system composed of similar particles, that is, reduced to only one phase (of constant specific volume in our framework). By specializing the concept to a phase basis, we remove the ambiguity on which is the relevant velocity field to be used. Moreover, for potential energies depending only on the volume fraction, we can derive the corresponding force in exact math.

We start with the most common flux, the diffusion flux.



## 5.1 Derivation of standard diffusion from energy consideration

Let us consider the classical case of two gases in thermal and pressure equilibrium in separate volumes. Upon connecting the two volumes, both gas will mix until a constant volume fraction is reached everywhere for both gas. The pressure and temperature are conserved, so the gas total energy is unchanged, but the entropy of the system has increased. However, discernible macroscopic movement has been performed by each phase considered separately. How movement can appear without energy change? What is the energy that the single phase is trying to minimize?

We have to consider the change of internal energy with the concentration. In [7], the chemical potential depends on the concentration with a logarithmic law. In the case of a mixture of perfect gases, the chemical energy  $G_a$  of phase A reverts the form of a thermal energy:

$$G_a = \int (nkT) a \ln a \quad (112)$$

where (only) here  $n$  is the volumetric number of molecules,  $k$ , the Boltzmann constant and  $T$  the temperature. Here,  $(nkT)$  is considered constant. We can infer the force derived from this energy:

$$d_t G_a(u_a) = \int_{\Omega} (nkT) \partial_t a \ln a = (nkT) \int_{\Omega} (\ln a + 1) \partial_t a \quad (113)$$

$$\begin{aligned} &= -(nkT) \int_{\Omega} (\ln a + 1) \nabla \cdot a u_a = (nkT) \int_{\Omega} \nabla [(\ln a + 1)] a u_a \\ &= \left\langle \frac{(nkT)}{a} \nabla a, a u_a \right\rangle_{L^2} \end{aligned} \quad (114)$$

and accordingly, the corresponding force in the momentum equation of phase A should be:

$$F_a = -(nkT) \nabla a. \quad (115)$$

The corresponding force in the momentum equation of phase B, in turn, should be

$$F_b = -(nkT) \nabla b \quad (116)$$

such that their sum cancels in the overall momentum equation. In the case of non perfect gases, the expression of the relevant part of the chemical potential is likely to change and if the forces do not sum anymore to zero, then their resultant should be added to global momentum equation. For gases, the forces tend to push the phases in the direction of smaller concentration and

are therefore strongly related to inter-diffusion. The important point here is to note that the diffusive flux according to Fick's law is proportional to  $F_a$ . This kind of relation will be clarified later.

For arbitrary small volume fraction, the specific volumetric chemical energy density becomes (slowly) infinite. However, an arbitrary small smooth (continuous) volume fraction has clearly lost meaning when, say, there is less than one molecule in the physical system under study. If surface tension arises from a bounded specific volumetric energy density for low volume fraction, then it will never totally cancel the diffusion effect. This is consistent with the concept of strictly positive (but eventually very small) vapour pressure. For numerical completely immiscible fluids, the force arising from the thermal part of the chemical potential should be however completely ignored.

## 5.2 Gravitational potential

To comfort ourselves with the methodology, we apply it to the gravitational potential  $E_g = \int \rho g z$ . We consider that the potential gravitational is (obviously) split among the phases according to the scheme:

$$E_g = E_{ga} + E_{gb} \quad (117)$$

$$E_{ga} = \int a \rho_a g z \quad (118)$$

$$E_{gb} = \int b \rho_b g z. \quad (119)$$

Then, direct calculation gives:

$$d_t E_{ga} = \int \partial_t a \rho_a g z = \langle a \rho_a g n_z, u_a \rangle_{L^2} \quad (120)$$

$$d_t E_{gb} = \int \partial_t b \rho_b g z = \langle b \rho_b g n_z, u_b \rangle_{L^2} \quad (121)$$

$$d_t E_g = \int \partial_t \rho g z = \langle \rho g n_z, u \rangle_{L^2}. \quad (122)$$

leading to the forces:

$$F_{ga} = -a \rho_a g n_z \quad (123)$$

$$F_{gb} = -b \rho_b g n_z \quad (124)$$

$$F_g = -\rho g n_z. \quad (125)$$

having the conservative properties:

$$F_{ga} + F_{gb} = F \quad (126)$$

and

$$F_{ga} u_a + F_{gb} u_b = F u \quad (127)$$

consistent with the usual gravitational force in the momentum equation.

As is written in thermodynamics books [7, 9], gravity does not cause diffusion by itself. One may object that many mixtures of different density tend to segregate under common experimental conditions. However, we do not expect such segregation to occur under free fall condition. The segregation is not directly due to gravity but rather to the induced pressure gradient.

We have seen before that the forces derived from the chemical potentials have diffusion effects and cancel each other by summation in the global momentum equation. As now we are confronted with an energy leading to perfectly summing forces and corresponding to no diffusion effects, we may wonder whether this dichotomy is general or not.

### 5.3 Pressure shift

While surface tension importance is noteworthy at millimetre range and greater at smaller scale, pressure gradient is also noteworthy at millimetre range but is greater at higher scale. Typically, the greater the droplet or bubble size, the greater its terminal velocity under a gravity induced pressure gradient. While in the millimetre range, a bubble or droplet under gravity pressure gradient is almost spherical, indicating a dominant surface tension effect, in the centimetre range, bubbles and droplets tend to deform and eventually break. As we are interested in free-surface flows with a resolved scale of a few millimetres, we should take into consideration both surface tension and pressure differential effects. What we want to obtain is the spontaneous separation of a flow at rest with an initial homogeneous intermediary volume fraction. The shift direction of the heavy phase should be in the resolved pressure gradient direction. The shift direction of the light phase should be opposite to the resolved pressure gradient direction. There are so many ways two fluids can inter-penetrate at a given macroscopic scale that it is unrealistic to hope solving the drift velocity issue consistently with all of these ways. In effect, the microscopic distribution of the two phases has normally a very large impact on the drift velocity. For example, a light phase volumetric density of 0.001 in a 1mm cubic cell can be resolved with one unique spherical bubble about 0.1 mm in linear size, with one thousand bubbles size 0.01 mm, with mixing at molecular level or with a cylindrical tube 1mm long and 0.03mm large. The position of the structures needs not to be evenly distributed. In each case, the drift velocity is quite different.

In our case, the main cause of mixing is numerical diffusion, not physical in nature, and we can just decide the internal structure of the mixing if it can help for building counter-measures. We will build our pressure shift on a

mixing structure similar to the molecular mixing, but not constrained by the molecular scales.

In all two phase flow models the pressure gradient appears as  $a\nabla P$  in the phase A momentum equation and as  $b\nabla P$  in the phase B momentum equation, so that the two terms consistently sum to  $\nabla P$  in the global momentum equation.

If we suppose that these pressure gradient forces are derived from two energies  $E_a$  and  $E_b$  then their variations are:

$$d_t E_a = \langle a\nabla P, u_a \rangle_{L^2} = \langle -P, \nabla \cdot a u_a \rangle_{L^2} \quad (128)$$

$$d_t E_b = \langle b\nabla P, u_b \rangle_{L^2} = \langle -P, \nabla \cdot b u_b \rangle_{L^2} \quad (129)$$

The corresponding energies are  $E_a = aP$  and  $E_b = bP$  but with the time dependency of the pressure ignored. In the incompressible framework, it is known that the pressure is defined only up to a constant. This constant is constant only in space but not necessarily in time. Let us call  $P_0(t)$  this function of time and choose:

$$E_a = a(P + P_0(t)) \quad (130)$$

then a straightforward calculation gives:

$$d_t E_a = \langle a\nabla P, u_a \rangle_{L^2} + \partial_t P_0(t) \int_{\Omega} a + \int_{\Omega} a \partial_t P. \quad (131)$$

Writing  $V_a = \int_{\Omega} a$  (which is for our concern time invariant), by choosing  $P_0(t)$  to be precisely:

$$P_0(t) = \frac{-1}{V_a} \int_{\Omega} a \partial_t P, \quad (132)$$

then we have exactly:

$$d_t E_a = \langle a\nabla P, u_a \rangle_{L^2} \quad (133)$$

and the pressure gradient term is made to derive directly from a time dependent potential.

The pressure gradient forces do not behave neither as the gravity (summing perfectly) nor as the thermal agitation force (summing to zero). We can however try to split each phase force in two parts: one behaving like gravity and the other one behaving like a momentum exchange. This is the argument of the following part.

## 6 Dynamic equilibrium assumption

We have seen that when an energy is involved in a two phase flow, it is important to understand how we can split this energy between the two phases. The force derived on the global flow will heavily depend on this splitting. We have already encountered two particular cases: the gravity potential and the thermal part of the chemical potential. The gravity potential works ideally in the sense that the potential of the mixture is associated to a force which is the sum of the forces associated the phase potentials. On the contrary, the chemical potential (considered before) is such that the sum of the forces applied to the single phases cancels identically.

When a generic force  $F$  is present in the mixture momentum equation, it is always possible to split the force among the phase momentum equations such that the phase forces behave like gravity. We just have to do the splitting:

$$F_a = \frac{a\rho_a}{\rho} F \quad (134)$$

$$F_b = \frac{b\rho_b}{\rho} F, \quad (135)$$

such that

$$F_a + F_b = F \quad (136)$$

$$F_a u_a + F_b u_b = F u. \quad (137)$$

On the other hand, we do not know if the splitting is correct because we can add to the phase forces whatever pair of opposite forces.

Now, from the viewpoint of the phases, given a pair of forces related by some physical meaning, we can wonder which part of the force pair behaves like gravity and which part sums to identically vanish. It turns out that the splitting can be done generically and is quite easy to perform. In effect, taking profit of the former splitting, we just have to invert the system:

$$F_a = \frac{a\rho_a}{\rho} F + F_0 \quad (138)$$

$$F_b = \frac{b\rho_b}{\rho} F - F_0 \quad (139)$$

giving

$$F = F_a + F_b \quad (140)$$

$$F_0 = \frac{b\rho_b}{\rho} F_a - \frac{a\rho_a}{\rho} F_b. \quad (141)$$

As a typical example, we have the pressure based force for the phases  $F_a =$

$-a\nabla P$  and  $F_b = -b\nabla P$ . We find:

$$F = -\nabla P \quad (142)$$

$$F_0 = -\frac{ab(\rho_b - \rho_a)}{\rho} \nabla P. \quad (143)$$

Note that  $F$  would have been the same taking  $F_a = -\nabla aP$  and  $F_b = -\nabla bP$ .

The splitting performed here is now interpreted in the following way. The summing part of the force can work to move the whole mixture while the work of the cancelling part is lost against friction with the other phase. Consequence of this interpretation is that we do not need to know the cancelling part of the forces to build the mixture momentum equation. A second and the most important consequence of this interpretation is that the cancelling part of the forces is strongly related to the rate of exchange of momentum with the other phase.

Our modelling assumption is that the cancelling part of the forces is properly in dynamical equilibrium with the rate of exchange of momentum with the other phase. That is:

$$F_0 = I_b. \quad (144)$$

As we model the momentum exchange with a term proportional to the velocity difference, the velocity difference is known up to this coefficient of proportionality. As the corrective flux is also proportional to the velocity difference, it is also defined up to the same coefficient of proportionality.

To check the validity of this interpretation, we can inquire whether we can retrieve some known results. First, we retrieve that gravity by itself does not induce diffusion. Second, the concentration diffusion directly follows from the term  $-P\nabla a$  foreseen inside the force  $F_a$  for perfect gases ( $P = -(nkT)$ ). Third, the baro-diffusion, following from the  $a\nabla P$  part of the phase pressure term operates only in presence of a density difference.

These three results seem consistent with the derivations given in [7]. Conversely, the last two results confirm the presence of  $\nabla aP$  as phase A pressure term for perfect gases. Once reduced, the phase equations could look like:

$$\partial_t a \rho_a u_a + \nabla \cdot a \rho_a u u_a + \frac{a \rho_a}{\rho} \nabla \cdot [PI + \tau] = a \rho_a g + \frac{a \rho_a}{\rho} F, \quad (145)$$

$$\partial_t b \rho_b u_b + \nabla \cdot b \rho_b u u_b + \frac{b \rho_b}{\rho} \nabla \cdot [PI + \tau] = b \rho_b g + \frac{b \rho_b}{\rho} F, \quad (146)$$

where  $F$  stands for any additional force which should appear in the global momentum equation, letting room to the coming surface tension. We have also applied the hypothesis that the partial pressure tensor is unitary in the mass weighted velocity reference frame.

The dynamic equilibrium condition reads:

$$Rab(u_b - u_a) = \frac{ab(\rho_b - \rho_a)}{\rho} \nabla P - F_0 \quad (147)$$

leading directly to the expression of the diffusive fluxes.

## 6.1 Extension to other internal phenomena

In the previous subsection, we have seen that the classical diffusion can be reinterpreted as a force derived from an energy and acting separately on each phase and whose sum identically cancels so as to give no contribution to the overall momentum equation.

It could be interesting to investigate which are the energies whose derived force applied separately on each phase have their sum cancel identically in the overall momentum equation. In this approach, we postulate that the overall momentum equation can be built (as we have just done) by summing the single phase momentum equations. Moreover, we would not need to know the exact form of the single phases momentum equations, but only the expression of the forces acting in it.

Let an energy  $E_a$  of phase A be the volume integral of an energy density  $e_a$  depending only algebraically on the volume fraction  $a$ , and not on its derivative.

$$E_a = \int e(a). \quad (148)$$

We use the representation:

$$\partial_t E_a = \langle -F_a, u_a \rangle_{L^2} \quad (149)$$

and the transport equation of phase A:

$$\partial_t \rho_a a = -\nabla \cdot \rho_a a u_a. \quad (150)$$

As we restrict our analysis to cases in which the phase densities are constant, the later equation reduces to:

$$\partial_t a = -\nabla \cdot a u_a. \quad (151)$$

The domain of integration being fixed, we can easily compute the time evolution of the energy  $E_a$ :

$$\partial_t E_a = \int \partial_t e(a) = \int e'(a) \partial_t a \quad (152)$$

$$= - \int e'(a) \nabla \cdot a u_a = \langle a \nabla e'(a), u_a \rangle_{L^2} \quad (153)$$

$$\partial_t E_a = \langle a e''(a) \nabla a, u_a \rangle_{L^2}. \quad (154)$$

Leading to:

$$F_a = af_a = -ae''(a)\nabla a. \quad (155)$$

The force  $F_a$  should appear in the phase A momentum equation, that is the equation giving  $\partial_t a \rho_a u_a$ , the global momentum equation being constructed by summing this term for both phases. The reduced force  $f_a$  would be the term appearing in an hypothetical evolution equation for  $\partial_t \rho_a u_a$ .

Now, we suppose that phase B has an energy  $E_b$  which can be represented by the same energy density  $e$ , however applied to phase B:

$$E_b = \int e(b). \quad (156)$$

repeating the former derivation, we get:

$$F_b = bf_b = -be''(b)\nabla b = be''(b)\nabla a. \quad (157)$$

We want to know how we can choose the energy density  $e$  such that  $F_a + F_b = 0$ . We have:

$$F_a + F_b = af_a + bf_b = [be''(b) - ae''(a)]\nabla a. \quad (158)$$

That is, unless we discard the perfectly mixed case which is not of our current interest, we must solve:

$$be''(b) - ae''(a) = 0. \quad (159)$$

Clearly, the solutions of this equation form a vectorial space containing the affine functions, as  $e(x) = \alpha x + \beta$  is a trivial solution. Another, maybe complete, set of solution is obtained by solving:

$$e''(a) = bg(ab) \quad (160)$$

for whatever algebraic function  $g$ .

Taking  $g(ab) = \frac{g_0}{ab}$  we get, up to an affine function:

$$e(a) = g_0 a \ln a \quad (161)$$

and we retrieve the energy at the origin of the classical diffusion.

Scanning  $g$  functions for potentially interesting candidates, we find  $g(ab) = g_0$ , giving by fixing the integration constants:

$$e(a)'' = g_0 b = g_0(1 - a) \quad (162)$$

$$e(a)' = g_0 \left( \frac{-a^2}{2} + a - \frac{1}{3} \right) \quad (163)$$

$$e(a) = \frac{-g_0}{6} (a^3 - 3a^2 + 2a) = \frac{-g_0}{6} a(1 - a)(2 - a) \quad (164)$$

$$e(a) = \frac{-g_0}{6} ab(1 + b) \quad (165)$$



and

$$F_a = g_0 ab \nabla a. \quad (166)$$

We shall see that this force is an excellent candidate for a contracting term. By the way, other candidates can be tested, but we could not find any other one leading to simple expressions.

## 6.2 Extension of the derivation of the surface tension from energy consideration

We have now in hands the necessary tools required to extend the derivation of the surface tension for two constant density fluids which can inter-penetrate.

Let us postulate a free energy  $G$  to be globally minimized by the flow in the form:

$$G = \int_{\Omega} \sigma |\nabla H(a)| \quad (167)$$

where now for simplicity, the surface tension coefficient is considered constant and  $H$  is a normalised monotonous (increasing) scalar function with (positive) derivative  $h$ . We recall the volume fraction equation:

$$\partial_t a + \nabla \cdot (a u_a) = 0 \quad (168)$$

The velocity used in the momentum equation is  $u$  and we would like to apply the representation:

$$d_t G = \langle -F, u \rangle_{L^2(\Omega)} \quad (169)$$

with the scalar product on the right hand side classically defined in our case as:

$$\langle f, g \rangle_{L^2(\Omega)} = \int_{\Omega} f g. \quad (170)$$

We just have therefore to evaluate,  $d_t G_u$  and represent it, if feasible, under the form  $\langle -F, u \rangle_{L^2(\Omega)}$ . This representation arises from the conservation of the total energy when the kinetic energy is  $E_c = \int_{\Omega} \frac{\rho}{2} u^2$ . Unfortunately, in presence of two phases, the total kinetic energy is rather:

$$E_c = \int_{\Omega} \frac{a \rho_a}{2} u_a^2 + \frac{b \rho_b}{2} u_b^2 = \int_{\Omega} \frac{\rho}{2} u^2 - \frac{ab \rho_a \rho_b}{2\rho} (u_a - u_b)^2 \quad (171)$$

and the two expressions differ when the phase velocities are not equal. However, the representation is correct if applied on a single phase basis.

The domain of evaluation  $\Omega$  does not change in time and we can write:

$$d_t G = \int_{\Omega} \partial_t(\sigma |\nabla H(a)|) \quad (172)$$

$$= \int_{\Omega} \sigma n \nabla \partial_t H(a)$$

$$d_t G = - \int_{\Omega} \sigma n \nabla [h \nabla \cdot a u_a] \quad (173)$$

$$= - \langle a \nabla [h \nabla \cdot \sigma n], u_a \rangle_{L^2} \quad (174)$$

$$= \langle b \nabla [h \nabla \cdot \sigma n], u_b \rangle_{L^2} . \quad (175)$$

depending on to which velocity the force must be set in duality with, we obtain:

$$F_a = a \nabla [h \nabla \cdot \sigma n] \quad (176)$$

if the energy has to be considered a property of phase A and

$$F_b = -b \nabla [h \nabla \cdot \sigma n] \quad (177)$$

if the energy has to be considered a property of phase B.

We can proceed with the derivation for further insight

$$d_t G = - \int_{\Omega} \sigma n \nabla [h \nabla \cdot a v + a b (u_a - u_b)] \quad (178)$$

$$= \int_{\Omega} (h \nabla \cdot \sigma n) (v \cdot \nabla a + \nabla \cdot a b (u_a - u_b))$$

$$= \langle \nabla \cdot (\sigma n) \nabla H(a), v \rangle_{L^2(\Omega)} + \langle h \nabla \cdot (\sigma n), \nabla \cdot a b (u_a - u_b) \rangle_{L^2(\Omega)}$$

$$d_t G_u = \langle \nabla \cdot (\sigma n) \nabla H(a), v \rangle_{L^2(\Omega)} \quad (179)$$

$$- \langle \nabla h \nabla \cdot (\sigma n), a b (u_a - u_b) \rangle_{L^2(\Omega)}$$

We retrieve the classical surface tension under the condition that the shift velocity  $u_a - u_b$  is null, however in duality with the volume fraction velocity. We are thus here in perfect agreement with the surface tension defined by Landau, under the condition (required in the development of Landau) that the phases are completely separated, and thus  $u$  and  $v$  are equal.

We are apparently in a very favourable situation in which the initial target form can be reached. It is not very intuitive to arrive to the right form, but once found, it is straightforward to derive it directly. We start with the decomposition:

$$\rho u = a \rho_a u_a + b \rho_b u_b \quad (180)$$

$$= (\rho_a - \rho_b) a u_a + a \rho_b u_a + b \rho_b u_a \quad (181)$$

$$= (\rho_a - \rho_b) a u_a + \rho_b v. \quad (182)$$

Remembering that  $v$  is divergence free, we have directly:

$$\nabla \cdot au_a = \nabla \cdot \frac{\rho u}{\rho_a - \rho_b} \quad (183)$$

and making the substitution in equation 173, it comes after integration by parts:

$$d_t G_u = < -\frac{\rho}{\rho_a - \rho_b} \nabla [h(\nabla \cdot \sigma n), u] >_{L^2(\Omega)} . \quad (184)$$

or to make the classical force appear:

$$\begin{aligned} d_t G &= < \nabla \cdot (\sigma n) \nabla H(a), u >_{L^2(\Omega)} \\ &- < \nabla [(\nabla \cdot \sigma n) \frac{\rho h}{\rho_a - \rho_b}], u >_{L^2(\Omega)} . \end{aligned} \quad (185)$$

The force related to the duality with the mass weighted velocity is therefore:

$$F = \frac{\rho}{\rho_a - \rho_b} \nabla [h \nabla \cdot \sigma n] \quad (186)$$

Note that this derivation does not apply when both densities are equal. This is because we have deeply used the fact that density and volume fractions have collinear gradients.

If we consider that the energy density  $g = \sigma |\nabla H(a)|$  is split among the two phases according to the scheme:

$$g = g_a + g_b \quad (187)$$

$$g_a = \frac{\rho_a}{\rho_a - \rho_b} \quad (188)$$

$$g_b = -\frac{\rho_b}{\rho_a - \rho_b}, \quad (189)$$

and naming  $F_a, F_b$  and  $F$  the forces related to the pairs  $(g_a, u_a), (g_b, u_b)$  and  $(g, u)$ , then we retrieve the expected additive properties:

$$F_a + F_b = F \quad (190)$$

and

$$F_a u_a + F_b u_b = F u. \quad (191)$$

The force thus obtained is not very different from the classical one. In effect, part integration gives:

$$\begin{aligned} F &= \nabla \left[ \frac{\rho}{\rho_a - \rho_b} \nabla \cdot \sigma n \right] \\ &- \nabla \cdot [\sigma n] \nabla a. \end{aligned} \quad (192)$$

The first RHS term could be absorbed in the pressure gradient. The second RHS term coincides with the classical surface tension force. The derivation of

the force is correct, but the physical principal on which it is based is slightly wrong, leading to the degeneracy of the first RHS term when the densities are arbitrarily close.

As we want to extend the surface tension consistently to cases in which the interface width is non zero due to the discretisation of the equations, we would definitively prefer to keep the classical term  $F = -\sigma \nabla \cdot n \nabla H(a)$  without any change. This cannot be achieved by a simple global weighting of the phase forces already defined. It can nevertheless be achieved using a less trivial splitting of the energy between the phases. In effect, taking:

$$E_a = \int \sigma |b \nabla a| \quad (193)$$

$$E_b = \int \sigma |a \nabla b| \quad (194)$$

we still have  $E_a + E_b = \int \sigma |\nabla a|$ , but in this case the (normalized) forces are:

$$F_a = \nabla [ab \nabla \cdot n] - b \nabla \cdot n \nabla a \quad (195)$$

$$F_b = -\nabla [ab \nabla \cdot n] - a \nabla \cdot n \nabla a. \quad (196)$$

As the forces do not perfectly sum, we can expect diffusion-like induced phenomena for the phases. We shortly comment on this feature.

We want to extend the energy concept for cases in which two phases can merge. However, we want that the two phases tend to separate. This is not realized with the energy  $G = \int_{\Omega} \sigma |\nabla a|$  as can be seen from two specific cases. First, if the phases are (vertically) stratified, the energy is invariant with the stratification width. Second, for the situation in which the phase A is restricted to a single sphere, for a given total volume of phase A, the energy decreases with the enlarging of the sphere and a related lowering of the volume fraction (supposed constant but no more unit) in the sphere. Taking  $S$  the surface of the spheres, we have:  $G_1 = \sigma S_1$  and  $G_a = a S_a = a^{1/3} S_1 \leq S_1$ .

This means that this energy favours the dissolution of droplets or bubbles. In fact, the lowest energy is reached for a uniform mixing of the phases.

Now, we look at  $F_0$  the cancelling part of phase A force:

$$F_0 = \frac{b\rho_b}{\rho} F_a - \frac{a\rho_a}{\rho} F_b \quad (197)$$

$$= \frac{ab}{\rho} \nabla (\rho \nabla \cdot n) \quad (198)$$

$$= ab \nabla (\nabla \cdot n) + \frac{ab(\rho_a - \rho_b)}{\rho} (\nabla \cdot n) \nabla a \quad (199)$$

$$F_0 = ab \nabla (\nabla \cdot n) - \frac{ab(\rho_a - \rho_b) F}{\rho} \quad (200)$$

For spherical bubbles or droplets,  $\nabla(\nabla \cdot n)$  is oriented in direction of  $-n$ . The first RHS term in equation (199), which is the only one present in case of constant density, induces a diffusive behaviour. This term is consistent with the previous comment. In more complex configuration, the force seems to work at the regularization of the curvature, but the interpretation is neither easy nor simple to justify. The second RHS term is similar to the corresponding pressure force with  $-F$  instead of  $\nabla P$ . It cancels the pressure drift effect for the part relative to the pressure change across the interface. It states that there is no pressure drift if the pressure gradient is due to a curvature induced surface tension. This effect seems to make sense, at least for CFD applications.

The original surface tension term has been retrieved using a symmetrical splitting of the energy between the two phases. In the case of a liquid/ low density gas interface, this splitting seems rather un-physical as we understand the surface tension as a property almost exclusively of the liquid phase. In this case, writing:

$$F_a = a\nabla[h\nabla \cdot n] = (\nabla \cdot n)\nabla(ah - H) + ah\nabla(\nabla \cdot n), \quad (201)$$

we must have  $h = 0$  when  $b = 0$ , otherwise the resulting force is diffused and depends on the prolongation of  $\nabla \cdot n$  all over the domain even in the regions where the product  $ab$  is identically zero. Thus, taking  $h$  proportional to  $b$  remains an interesting choice. Another advantage is the following: when the interface width is small in confront with the curvature radius, if the volume fraction gradient is constant across the interface, then the force is proportional to the heavy phase volume fraction and thus almost proportional to the density. We believe that this property reduces the stiffness of the equation if we require the volume fraction to be the smoother field, by opposition to the mass fraction more adequate for diffusive phenomena.

Up to the quite fastidious parasite diffusion effects, we would have found out a good energy term from which to derive the surface tension. Once again, to complete the current development we will have to settle and refine a few concepts.

### 6.3 Extension of the notion of surface density

To solve the issue of the diffusing effect arising from the current energy density used to describe the surface tension, we must refine the concept of interface density. While for completely separated media, it is correctly defined by  $|\nabla a|$ , for slightly inter-penetrating media, the definition cannot be trivially extended. Considering a planar interface, we must give an interface definition

such that the diffuse interface is larger than a wide-less one. One way is to weight the interface density with a positive function,  $W$ , characteristic of the diffuse region. The simplest function is the density product  $ab$ . It has also the nice property that it leads to a potential not modifying the global momentum equation. There is however arbitrariness in this choice. For dimensional homogeneity, we must also introduce a length  $L$ , such that our definition of the surface density  $s$  becomes:  $s = |\nabla a| + W(\frac{ab}{L})$ . Fundamentally,  $W(x) = x^2$  is used in the Cahn-Hilliard and Allen-Cahn equations. But here we use  $W(x) = x$ .

When we were suggesting  $E = \int \sigma |\nabla a|$  as the energy responsible for surface tension, we were in fact thinking at the integral of the surface density  $E = \int \sigma s$ . The idea is straightforwardly extended to the extended notion of surface by looking at the effects of the extra term.

We have already made the splitting allowing to have the phase forces summing to zero.

$$E_a = \int \sigma \frac{ab(1+b)}{3L} \quad (202)$$

$$E_b = \int \sigma \frac{ab(1+a)}{3L} \quad (203)$$

and

$$F_a = \frac{2\sigma}{L} ab \nabla a \quad (204)$$

$$F_b = -\frac{2\sigma}{L} ab \nabla a. \quad (205)$$

An interpretation of  $e_a = \sigma \frac{ab(1+b)}{3L}$  can be the following. First  $e_a$  is proportional to the particle number density, itself proportional to the volume fraction. The energy for each particle is then proportional to  $b(1+b)$ . The first  $b$  in this expression is to state that the augmented energy is roughly proportional to the lack of neighbours of the same phase A. The term  $1+b$  takes into account that the probability of a lacking neighbour to be a closest neighbour (associated with an higher energy) increases with the proportion of lacking neighbours. In other words, the local clustering of the particles drops with the volume fraction.

By comparison with the diffusive force arising from the main surface energy term, we can see that the combined effect is diffusive when  $|\nabla(\nabla \cdot n)| \geq \frac{2|\nabla a|}{L}$  and contracting otherwise.

Here again, the symmetrisation of the energy is very doubtful and difficult to justify for the gaseous light phase. Taking:

$$E = E_a = \int \sigma \frac{ab}{L} \quad (206)$$

we have

$$F = F_a = \frac{\sigma}{L} \nabla a^2. \quad (207)$$

The same result would have been obtained using  $E = E_a = \int -\frac{\sigma}{L} a^2$ , more easy to interpret as the sum of all binary connections between fluid molecules. This force creates a jump of pressure across the interface (independently of its curvature) equal to  $\frac{\sigma}{L}$ . This jump of pressure can be related to the internal pressure of the fluid which is normally filtered by the Navier-Stokes equations. The symmetrized splitting is thus to be interpreted as such a filtering. How much this interpretation can be extended to the symmetrisation of the previous term is left undecided.

## 6.4 Relation between potentials

A relatively general expression for the potential energy  $E$  at the source of the Cahn-Hilliard and Allen-Cahn equation rewritten with our notation is:

$$E = \int \frac{\alpha^2}{2} |\nabla G(a)|^2 + \frac{\beta^2}{2} f^2(ab) \quad (208)$$

with  $\alpha, \beta$ , two strictly positive coefficients,  $G$  a normalized function and  $g$  its derivative. Very often in literature,  $f$  and  $G$  are considered identity.

The question arises as whether there is a relation between this energy and the surface tension energy:

$$E' = \int \sigma |\nabla H(a)| \quad (209)$$

where here again  $H$  is a normalized function.

The answer lies in the elementary relation  $x^2 + y^2 \geq 2xy$  indicating that locally we have everywhere:

$$\frac{\alpha^2}{2} |\nabla G(a)|^2 + \frac{\beta^2}{2} f(ab)^2 \geq \alpha\beta fg |\nabla a|. \quad (210)$$

At the cost of having an extrinsic normalization of  $f$  such that  $fg \nabla a = \nabla H$ , setting  $\sigma = \alpha\beta$ , we have:  $E \geq E'$ . Moreover, we have  $E = E'$  if the Cahn-Hilliard energy density is everywhere minimum. And when it is minimum, both terms under the integral are equal, giving:  $\frac{|\nabla G|}{f} = \frac{\beta}{\alpha}$  from which the shape of the locally stable solution can be calculated.

When looking at the Cahn-Hilliard potential, we can see that the force derived from the scalar part has an integral across the interface which is independent of the interface curvature. The curvature dependent part of the force comes therefore exclusively from the gradient part of the potential and scales like  $\lambda^2 \alpha^2$ , where  $\lambda$  is the width of the interface. A consequence is

that the curvature effects due to the force derived from the Cahn-Hilliard potential can be very different from the surface tension effect, mainly when the resolved scale (i.e. in a CFD simulation) is much larger than the local equilibrium length scale  $\lambda_{eq} = \frac{\alpha}{\beta}$ , which is in the nanometre range except for fluid near the critical point [10].

We could modify the parameters  $\alpha$  and  $\beta$  in such a manner that their product is conserved but the equilibrium scale is much larger. If the modified equilibrium scale becomes resolved, then the surface tension should also be correctly resolved. Remark that in this case, the equilibrium shape of the interface must also be reasonably captured, requiring the resolved scale to be about one order less than the equilibrium scale. We would prefer not to have to resolve the interface shape and we would better have as objective an interface with only one or at most two cells or control values.

On the other hand, the force derived from the surface tension energy  $E'$  is almost insensitive to the resolved scale, as long as it is somewhat larger than the local curvature.

When a potential density must be expressed with a term containing the gradient of the volume fraction, then it automatically produces a force whose integral across the interface depends on the curvature. On the contrary, a potential depending only on the volume fraction gives rise to a force whose integral across the interface is independent of the curvature. Moreover, we have derived a family of such potentials which identically cancels when summed for the global momentum equation. These potentials are therefore perfectly suited for contracting purpose.

Our strategy to represent the surface tension effects has been to use the asymptotic potential  $E' = \int \sigma |\nabla H(a)|$  related to the classical surface tension force, and to augment it with a pair of mutually neutralizing phase potential for correction of unwanted diffusion effects.

The relation given here between the surface tension coefficient and the Cahn-Hilliard potential is not original and can be found in very similar terms in [10] (eq 3.13 pp.56). The relation between the surface tension and the degenerated potential can be found in Jacqmin 1999 [11].

## 6.5 Relation with the Cahn-Hilliard equation

The Cahn-Hilliard potential under examination is:

$$E = \frac{\sigma}{2} \int_{\Omega} \delta |\nabla a|^2 + \delta^{-1} a^2 b^2 \quad (211)$$

and we take both densities equal.



Supposing that the potential is a property of phase A (i.e.  $E = E_a$ ), we have straightforwardly:

$$F_a = \sigma a \nabla [\delta \Delta a - \delta^{-1} ab(b - a)] \quad (212)$$

$$F_0 = \sigma ab \nabla [\delta \Delta a - \delta^{-1} ab(b - a)] \quad (213)$$

thus the Cahn-Hilliard equation with a parameter dependent mobility is retrieved. Or, in alternative, we get back the constant mobility equation by modelling the resistance coefficient  $R$  in the momentum exchange term as proportional to the product  $ab$ . Such modelling assumption is however incompatible with a reasonable baro-diffusion. In both cases, we had not to suppose a negligible apparent velocity  $v$ .

The non gradient part of the force  $F_a$  appearing in the global momentum equation is proportional to  $-\Delta a \nabla a$  in clear correspondence with the surface tension.

## 7 Consequences for the numerical treatment of surface tension

The phase momentum equations were postulated mainly thinking to a perfect gas made of two species. To account for more general fluids, we have let the possibility to include some other arbitrary force. The application we have in mind concern an Heavy Liquid Metal (HLM), basically, Lead or Lead-Bismuth Eutectic (LBE) in contact with a low pressure gas. For some application, pressure is atmospheric, for some other application, pressure can be much less. We want to create a two-phase fluid model with some precise features.

- Both phases are incompressible
- When in diffuse form, each phase preserves its own density
- No phase diffuses spontaneously in the other
- When in diffuse form, the phases tend to spontaneously separate

These characteristic are required for CFD applications. The first one allows to use the general incompressible background. The second one expresses that when the phases mix, they mix as if they were gaseous phases. The third and fourth properties together state that the phases tend to be totally immiscible: under separated initial conditions, in exact mathematics, the fluid should stay separated for all time. This fluid is very much like the one used by [7] to derive the surface tension. It is not a Cahn-Hilliard fluid with a smooth transition between one phase and the other. However, the fluid will not evolve in a perfect mathematical world, but rather in an imperfect numerical (CFD)

world, more precisely in a Finite Volume (FV) CFD world without surface tracking mesh. In this world, the phases cannot evolve in space without suffering at least temporary broadening of their interface. Basically, during the filling of a new control volume, the phases are mixed in this control volume. Even at rest, the interface between the phases is technically (almost surely) wide at least one control volume. A more tricky situation arises when a fluid interface is driven (in one interface plane direction) from a coarse mesh region into a finer mesh region. In this case, the one broad cell large diffuse interface is convected in an interface region of several smaller cells. From these examples and others, one can infer that there are intrinsic sources of numerical diffusion of the interface, and that the numerical fluid is not in the configuration of a really immiscible fluid as required by the derivation of [7]. The distance to the ideal configuration and also the minimum distance to this ideal configuration evolve in time together with the flow. What we want to do is to incorporate a physical mechanism such that the evolving minimum distance is an attractor of the flow.

For us, the minimum distance is an interface one cell wide. It is unrealistic to try to define an articulated interface shape only one cell wide. Therefore, the objective shape will be the simplest one in this context: piece-wise linear. We want to base our additional force on an energy concept. As we have seen, to capture the surface tension effect almost independently of the interface width, we must rely on an energy density term of the form:

$$e_\sigma = \sigma |\nabla H(a)| = \sigma h(a) |\nabla a|. \quad (214)$$

according to equation 210, and following discussion, we must have  $f$  and  $g$  proportional to have the piecewise linear profile as reference. The simplest solution is therefore to take, once performed the normalization:

$$f = \chi_{ab} \quad (215)$$

$$h(a) = 1. \quad (216)$$

with  $\chi_{ab}$  the characteristic support function of the product  $ab$  (and also  $\lim_{\epsilon \rightarrow 0} (ab)^\epsilon$ ).

All curvature effects are supposed to be embedded in this energy density. The algebraic term in the Cahn-Hilliard potential is still needed to contract the interface width, with the difference that now the diffusive effects arise from the reduction of the available functional space due to the discretisation. We arrive to the following form of the global energy functional:

$$E_\rho = \int e_\sigma + e_c = \int \sigma |\nabla a| + \frac{\sigma}{L} ab \quad (217)$$

The length parameter  $L$  arises in a term dedicated to the control of discretisation effects, so it is likely that it will be defined according to parameters of the discretisation.

Now, we consider the nature of the two terms to understand how they should be split between the phases. The curvature effects are quite nicely described by the Landau expression. It is therefore very convenient to keep the same description for the extended configuration. Regarding the contracting term, it is an (anti-)diffusive term. We would like to treat it as an anti-diffusive force for each phase cancelling under summation in the global momentum equation. Its sole global effect is to generate drift fluxes. With both features available, we would have a global momentum equation perfectly unaltered. Thus, we choose:

$$e_{\sigma a} = be_{\sigma} \quad (218)$$

$$e_{\sigma b} = ae_{\sigma} \quad (219)$$

with the corresponding contracting forces:

$$F_{\sigma a} = \sigma[\nabla(ab\nabla \cdot n) - b(\nabla \cdot n)\nabla a] \quad (220)$$

$$F_{\sigma b} = \sigma[-\nabla(ab\nabla \cdot n) - a(\nabla \cdot n)\nabla a]. \quad (221)$$

such that the surface tension in the global momentum equation is:

$$F_{\sigma} = -\sigma(\nabla \cdot n)\nabla a \quad (222)$$

and the drift force for the phase transport equation is:

$$F_{\sigma 0} = \sigma ab\nabla(\nabla \cdot n) - \sigma \frac{ab(\rho_a - \rho_b)F}{\rho} \quad (223)$$

Regarding the contracting part, we have:

$$e_{ca} = \frac{\sigma}{3L}ab(1+b) \quad (224)$$

$$e_{cb} = \frac{\sigma}{3L}ab(1+a) \quad (225)$$

with the corresponding contracting forces:

$$F_{ca} = \frac{2\sigma}{L}ab\nabla a \quad (226)$$

$$F_{cb} = -\frac{2\sigma}{L}ab\nabla a. \quad (227)$$

from which the contracting drift fluxes are directly calculated taking  $F_0 = F_{ca}$  in equation (147).

## 8 Final system of equation

We resume the proposed set of equations.

Phase momentum equation:

$$\partial_t(a\rho_a u_a) + \nabla \cdot (a\rho_a u u_a) + a\nabla P - a\nabla \cdot \tau = I_{ab} + a\rho_a g + F_a \quad (228)$$

$$\partial_t(b\rho_b u_b) + \nabla \cdot (b\rho_b u u_b) + b\nabla P - b\nabla \cdot \tau = I_{ba} + b\rho_b g + F_b \quad (229)$$

with

$$F_a = F_{\sigma a} + F_{ca} \quad (230)$$

$$= \sigma a \nabla (b \nabla \cdot n) + \frac{2\sigma}{L} ab \nabla a \quad (231)$$

$$F_b = F_{\sigma b} + F_{cb} \quad (232)$$

$$= -\sigma b \nabla (a \nabla \cdot n) - \frac{2\sigma}{L} ab \nabla a \quad (233)$$

$$I_{ab} = -I_{ba} = Rab(u_b - u_a) \quad (234)$$

$$R = R_0(1 + |\delta \nabla a|^2) \quad (235)$$

Global momentum equation:

$$\partial_t(\rho u) + \nabla \cdot (\rho u u) + \nabla P + \nabla \cdot \tau = \rho g + F. \quad (236)$$

with

$$F = F_a + F_b = -\sigma(\nabla \cdot n)\nabla a \quad (237)$$

Volume fraction equations:

$$\partial_t a + \nabla \cdot (av) - \nabla \cdot [ab(u_b - u_a)] = 0, \quad (238)$$

$$\partial_t b + \nabla \cdot (bv) - \nabla \cdot [ab(u_a - u_b)] = 0. \quad (239)$$

in terms of the divergence free volume fraction velocity  $v$  and

$$\partial_t(\rho_a a) + \nabla \cdot (a\rho_a u) - \nabla \cdot \left[ \frac{ab\rho_a\rho_b}{\rho}(u_b - u_a) \right] = 0 \quad (240)$$

$$\partial_t(\rho_b b) + \nabla \cdot (b\rho_b u) + \nabla \cdot \left[ \frac{ab\rho_a\rho_b}{\rho}(u_b - u_a) \right] = 0. \quad (241)$$

in terms of the mass fraction velocity  $u$  used in the momentum equation, both velocities being related through the equation:

$$u - v = (\rho_b - \rho_a) \frac{ab}{\rho} (u_b - u_a) \quad (242)$$

Dynamical equilibrium assumption:

$$I_{ab} = \frac{b\rho_b}{\rho}(a\nabla P - F_a) - \frac{a\rho_a}{\rho}(b\nabla P - F_b) \quad (243)$$

$$= ab \frac{(\rho_b - \rho_a)}{\rho} (\nabla P - F) - ab\sigma \nabla (\nabla \cdot n) - ab \frac{2\sigma}{L} \nabla a. \quad (244)$$

The equilibrium equation can be factorized by the product  $ab$  and reduces to:

$$u_b - u_a = \frac{1}{R} \left[ \frac{(\rho_b - \rho_a)}{\rho} (\nabla P - F) - \sigma \nabla (\nabla \cdot n) - \frac{2\sigma}{L} \nabla a \right]. \quad (245)$$

If one does not want to bother with extremely fine characteristics of the surface tension derived diffusing effects, the corresponding fourth order term can be simply removed, leading to:

$$u_b - u_a = \frac{1}{R} \left[ \frac{(\rho_b - \rho_a)}{\rho} (\nabla P - F) - \frac{2\sigma}{L} \nabla a \right]. \quad (246)$$

Insertion of the equilibrium assumption in the phase momentum equation gives:

$$\partial_t(a\rho_a u_a) + \nabla \cdot (a\rho_a u u_a) + \frac{a\rho_a}{\rho} (\nabla P + \nabla \cdot \tau) = \frac{a\rho_a}{\rho} (\rho g + F) \quad (247)$$

$$\partial_t(b\rho_b u_b) + \nabla \cdot (b\rho_b u u_b) + \frac{b\rho_b}{\rho} (\nabla P + \nabla \cdot \tau) = \frac{b\rho_b}{\rho} (\rho g + F). \quad (248)$$

These equations can be factorized by their respective densities to give to phase velocity equations:

$$\partial_t(a u_a) + \nabla \cdot (a u u_a) + \frac{a}{\rho} (\nabla P + \nabla \cdot \tau) = \frac{a}{\rho} (\rho g + F) \quad (249)$$

$$\partial_t(b u_b) + \nabla \cdot (b u u_b) + \frac{b}{\rho} (\nabla P + \nabla \cdot \tau) = \frac{b}{\rho} (\rho g + F). \quad (250)$$

Summation of these later gives the volume fraction equation:

$$\partial_t(v) + \nabla \cdot (u v) + \frac{1}{\rho} (\nabla P + \nabla \cdot \tau) = g + \frac{F}{\rho}. \quad (251)$$

The only equation independent of time that we are able to construct to solve the pressure is by taking the divergence of this last equation. It is of the form:

$$\nabla \cdot \frac{\nabla P}{\rho} = \mathcal{F}. \quad (252)$$

The constraint to be respected by  $u$  is given by the divergence of equation (242) taking into account the dynamical equilibrium assumption and the equation of state  $\nabla \cdot v = 0$ .

## 9 Discussion

The initial objective of this work was to understand how two-phase flows with a generally identifiable free-surface interface could be consistently described. The hope was that with a clear representation of the phenomenology, we could

have insight on how to improve the quality of their numerical simulation and reach always higher density ratios.

When constructing the global momentum equation from the phase momentum equations, there is always a temptation to resolve inconsistencies by stating that the global equation is not completely valid for two phase flows. How much this assumption is true is left as an open question. Here, we have taken an alternative approach for which the global momentum equation is untouchable, including the surface tension as derived in Landau [7]. The global momentum equation is thus not altered. Terms are introduced in the volume fraction equation to consistently take into account barometric and surface tension effects. In the macroscopic flows of our interest, the barometric term is likely to be almost everywhere largely dominant. Ironically, pressure effects were primarily derived to understand how to proceed with the surface tension. In absolute mathematics, pressure diffusion, as already known and derived in [7], is relevant in only very specific applications, because the resistance coefficient is based on a molecular length scale. By analogy with the turbulent diffusion, larger scale baro-diffusion is likely to appear in turbulent flows as well as in flows discretised for CFD simulation, the corresponding length scale being related either to the turbulent length scale or to the mesh size. Baro-diffusion seems a very good candidate for the control of the free surface integrity.

The surface tension arises from a potential which is a degenerate configuration of a Cahn-Hilliard potential. We can use any of the potentials, but the Cahn-Hilliard one requires a much finer discretisation to describe the concentration evolution through the interface.

While it is not the primary objective of this work, we have developed a formalism allowing to combine phase separation process with baro-diffusion.

In the Cahn-Hilliard framework, curvature effects and phase separation effects are intimately merged. In our “augmented Landau” framework, each effect is controlled by a specific dedicated term. Quite surprisingly, the part of the potential responsible for the surface tension has a marginally diffusive effects. It has an effect on both the momentum and the phase transport equation. The effect on the phase transport equation can be likely neglected. The part responsible for the phase separation has no effect on the momentum equation but should not be forgotten for the phase transport equation. Thus, we can empower the phase separation effect without modifying (or even ignoring) the curvature effects.

For our applications, phase separation occurs essentially because of baro-diffusion. In very specific applications such as free fall jets, the baro-diffusion becomes totally ineffective. In this case, only the surface tension keeps the

phases separated. So, it is controlled by the sole surface tension separation term.

Most of the material presented here can hopefully be re-used in the framework of turbulent applications. The turbulence energy  $\rho\kappa$  appearing naturally in the equation could have its treatment share some similitude with the treatment of the pressure.

The extensive reference to various potential energies and their derived forces proved to be extremely powerful, once we understood that it is essentially restricted to the single phases. In this sense, gravity is rather tricky, because it can be applied indifferently to the phases separately or to the entire mixture. But it is a very specific case. Reverting to the classical Newton law of acceleration ( $F = m\gamma$ ), we can see that this law cannot be in general extended by summation to  $\Sigma F = (\Sigma m)\gamma$  unless the force is proportional to the mass. We think that this is essentially the reason why it is in general not justified to derive a force from a potential applying a displacement or a velocity indiscriminately to all components of a multi-component flow.

We hope that the work performed here will be used to increase consistently the range of CFD application dealing with high density ratio free surface flows.

Two particular features may result quite relevant. The first one is to take into account that the numerical flow does not need be divergence free but has a specified divergence which must be enforced at the projection step. The second feature is the introduction of a generic baro-diffusion term working at a natural separation of the phases. A strictly contracting term related to the chemical potential is likely to be added only when the level of description reaches the millimetre range.

## 10 Formula

The mass weighted  $u$  and volume weighted  $v$  velocities are related through the formula:

$$\rho(u - v) = (\rho_b - \rho_a)ab(u_b - u_a) \quad (253)$$

$$\rho = a\rho_a + b\rho_b. \quad (254)$$

Some other formula relating the different velocities are these:

$$u_a - u = \frac{b\rho_b(u_a - u_b)}{\rho} \quad (255)$$

$$u_b - u = \frac{a\rho_a(u_b - u_a)}{\rho} \quad (256)$$

$$u_a - v = b(u_a - u_b) \quad (257)$$

$$u_b - v = a(u_b - u_a). \quad (258)$$

The mass fraction defined by  $\rho\tilde{a} = \rho_a a$  has its differential:

$$d\tilde{a} = \frac{\rho_a \rho_b}{\rho^2} da \quad (259)$$

leading to the invariance property

$$\frac{da}{ab} = \frac{d\tilde{a}}{\tilde{a}\tilde{b}} \quad (260)$$

such that the diffusion coefficient according to Fick's law is equally easy to interpret in terms of volume or mass fractions.

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